*Supporting information for*

# Monomeric Thorium Dihydrido Complex: A Versatile Precursor to Actinide Metallacycles

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## Experimental Procedures

### General remarks

All reactions were carried out under a dry and oxygen-free nitrogen atmosphere using Schlenk techniques and a Vigor glovebox. The nitrogen in the glovebox was constantly circulated through a copper/molecular sieves (4 Å) catalyst unit. The oxygen and moisture concentrations in the glovebox atmosphere were monitored by $O_2$ (GE) / $H_2O$ (Xentaur) to ensure both were always below 0.1 ppm. Toluene, hexane and $Et_2O$ were purified by use of a Vigor VSPS-5 solvent purification system, and dried over fresh Na chips in the glovebox. THF and $C_6D_6$ were distilled from Na/K alloy/benzophenone ketyl, degassed by the freeze-pump-thaw method (three times), and dried over fresh Na chips in the glovebox. $ThCl_4(DME)_2$[1], $(Cp^{Ar^*})H$ ($Cp^{Ar^*}$ = $C_5Ar^*_5$; $Ar^*$ = 3,5-$^t$Bu$_2$-$C_6H_3$)[2] and (*E*)-1,4-diphenylbut-3-en-1-yne[3] were synthesized according to the published procedures. K(*p*-$CH_2$-$C_6H_4$-Me) was obtained from the reaction of n-BuLi with KO$^t$Bu in *p*-xylene, according to the previous procedure.[4] $KCp^{Ar^*}$ was generated in situ from the reaction of $(Cp^{Ar^*})H$ with excess KH in THF, and used directly after filtration. Other reagents were purchased and used without purification.

Samples for NMR spectroscopic measurements were prepared in the glovebox by use of J. Young valve NMR tubes. $^1$H and $^{13}$C NMR spectra were recorded on a Bruker AV400 or AV500 spectrometer. $^1$H and $^{13}$C NMR spectra of complexes were recorded using TMS as internal standard. The elemental analyses were performed on Elementar Vario EL cube ($WO_3$ was used as pro-oxidant) at National Analytical Research Centre of Changchun Institute of Applied Chemistry (CIAC). IR spectra were recorded on Nicolet iS5.

**Caution:** Natural thorium (primary isotope $^{232}$Th) is a weak $\alpha$-emitter (4.012 MeV) with a half-life of 1.41 x $10^{10}$ years; manipulations and reactions should be carried out in monitored fume hoods or in an inert-atmosphere glovebox in a laboratory equipped with $\alpha$- and $\beta$- counting equipment.

### Synthesis of [$(Cp^{Ar^*})$Th(*p*-$CH_2$-$C_6H_4$-Me)$_3$] (1).

$KCp^{Ar^*}$ (1.00 mmol) in 10 mL THF solution was added dropwise to a stirred solution of $ThCl_4(DME)_2$ (555 mg, 1.00 mmol) in THF (20 mL). The resulting slurry was stirred at room

temperature for 12 h. To the resulting pale-yellow slurry was added solid of K(*p*-$CH_2$-$C_6H_4$-Me) (433 mg, 3.00 mmol) in several portions, which afforded a yellow brown colored solution that was stirred at room temperature for 3 h. The mixture was then filtered through a Celite-padded coarse frit to remove the insoluble salts. The yellow brown filtrate was collected and the volatiles were removed under reduced pressure to give a yellow solid. This solid was extracted with hexane (2 x 5 mL). The obtained extract was concentrated to 3 mL, and kept at -30 °C to give **1** (855 mg, 0.55 mmol, 55% yields) as pale-yellow crystals. Single crystals of **1** · (2x$C_6H_{14}$) suitable for X-ray analysis, were grown from hexane at -30 °C. $^1$H NMR (400 MHz, $C_6D_6$): *δ* = 7.32 (s, 5H, $C_5Ar_5$), 7.27 (s,10H, $C_5Ar_5$), 7.12 (d, *J* = 7.8 Hz, 6H, $C_6H_4$), 6.35 (d, *J* = 7.9 Hz, 6H, $C_6H_4$), 2.25 (s, 9H, $C_6H_4$-*Me*), 2.11 (s, 6H, $CH_2$-$C_6H_4$), 1.16 (s, 90H, Ar-$^t$*Bu*). $^{13}$C{$^1$H} NMR (101 MHz, $C_6D_6$): *δ* = 149.89 ($C_5Ar_5$), 139.24 ($C_6H_4$), 135.33 ($C_5Ar_5$), 132.97 ($C_6H_4$), 132.78 ($C_5Ar_5$), 131.47 ($C_6H_4$), 128.37 ($C_6H_4$), 127.13 ($C_5Ar_5$), 120.18 ($C_5Ar_5$), 87.67 ($CH_2$-$C_6H_4$), 34.78 ($C(CH_3)_3$), 31.52 ($C(CH_3)_3$), 20.75 ($C_6H_4$-*Me*).FT-IR (KBr, cm$^{-1}$): 3719, 3605, 3063, 2964, 2904, 2868, 1743, 1592, 1516, 1477, 1393, 1362, 1288, 1249, 1202, 1165, 1119, 1070, 934, 910, 899, 875, 795, 776, 712. Anal. calcd. for (**1**) $C_{99}H_{132}Th_1$ (1554.08): C, 76.51; H, 8.56; found: C, 77.12; H, 8.81.

**Synthesis of [($Cp^{Ar*}$)($Cp^*$)$ThH_2$(THF)] (2).**

In the glovebox, [($Cp^{Ar*}$)Th(*p*-$CH_2$-$C_6H_4$-Me)$_3$] (**1**) (775 mg, 0.5 mmol) and ($Cp^*$)H (68.0 mg, 0.5 mmol) in THF (5 mL) were charged into a glass tube in a medium-pressure autoclave with a magnetic stirring bar. The autoclave was transferred outside of the glovebox and pressurized with $H_2$ to 10 atm. The mixture was stirred at room temperature for 12 h. Pressure was released and the autoclave was quickly returned to the glovebox. After filtration, all the volatiles were removed under vacuum. The residue was washed with cold hexane (1 mL) and dried under vacuum to give **2** (680 mg, 0.47 mmol, 94% yield) as a white solid. Single crystals of **2** · (1.5x$C_6H_{14}$) suitable for X-ray analysis, were grown from hexane at -30 °C. $^1$H NMR (500 MHz, $C_6D_6$): *δ* = 23.47 (s, 2H, Th-*H*), 7.27 (s, 5H, $C_5Ar_5$), 7.24 (s, 10H, $C_5Ar_5$), 3.69 (br, 4H, *THF*), 2.47 (s, 15H, $C_5Me_5$), 1.46~1.38 (m, 4H, *THF*), 1.16 (s, 90H, Ar-$^t$*Bu*).$^{13}$C{$^1$H} NMR (126 MHz, $C_6D_6$): *δ* = 150.11 ($C_5Ar_5$), 135.67 ($C_5Ar_5$), 134.22 ($C_5Ar_5$), 127.30 ($C_5Ar_5$), 125.61 ($C_5Me_5$), 119.99 ($C_5Ar_5$), 70.11 (*THF*), 35.02 ($C(CH_3)_3$), 31.84 ($C(CH_3)_3$), 26.29 (*THF*), 13.02 ($C_5Me_5$).

FT-IR (KBr, $cm^{-1}$): 3657, 3061, 2964, 2905, 2868, 1770, 1592, 1537, 1477 1392, 1362, 1298, 1248, 1202, 1082, 933, 910, 898, 875, 712. Anal. calcd. for (**2**) $C_{89}H_{130}O_1Th_1$ (1447.96): C, 73.82; H, 9.05; found: C, 74.42; H, 9.51.

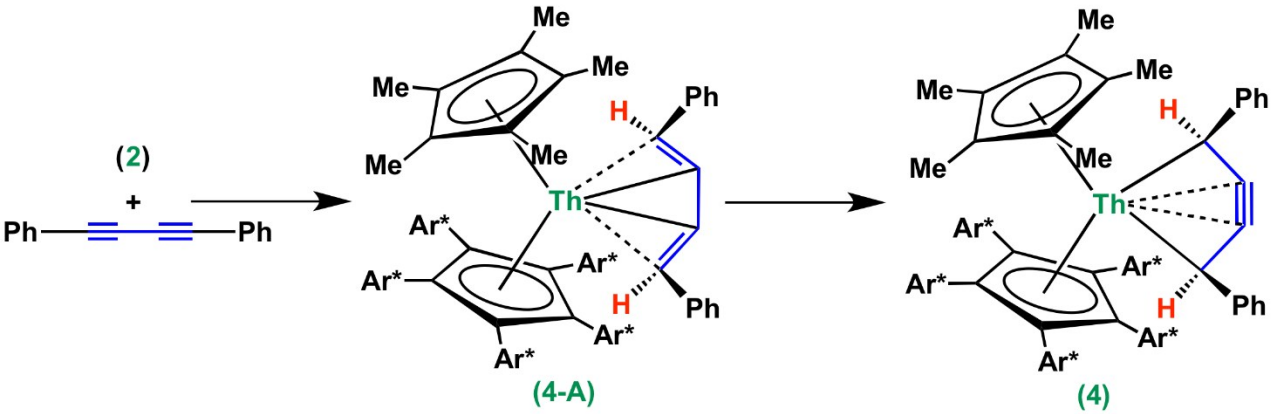
**Synthesis of [($Cp^{Ar*}$)($Cp^{*}$)$ThD_2$(THF)] (2-D).**

In the glovebox, [($Cp^{Ar*}$)($Cp^{*}$)$ThH_2$(THF)] (50 mg) in $C_6D_6$ (1 mL) were charged into a glass tube in a medium-pressure autoclave. The autoclave was transferred outside of the glovebox and pressurized with $D_2$ to 10 atm. The mixture was stirred at room temperature for 5 days. Pressure was released and the autoclave was quickly returned to the glovebox. The product had a $^1$H NMR spectrum which was identical with complex **2** except the low-field hydride resonance was missing. FT-IR (KBr, $cm^{-1}$): 3656, 3063, 2964, 2905, 2867, 1743, 1592, 1533, 1477, 1392, 1362, 1249, 1202, 1080,1027 (Th-D), 999 (Th-D), 933, 910, 898, 873, 712.

**Synthesis of [($Cp^{Ar*}$)($Cp^{Me4}$)$ThH_2$(THF)] (3).**

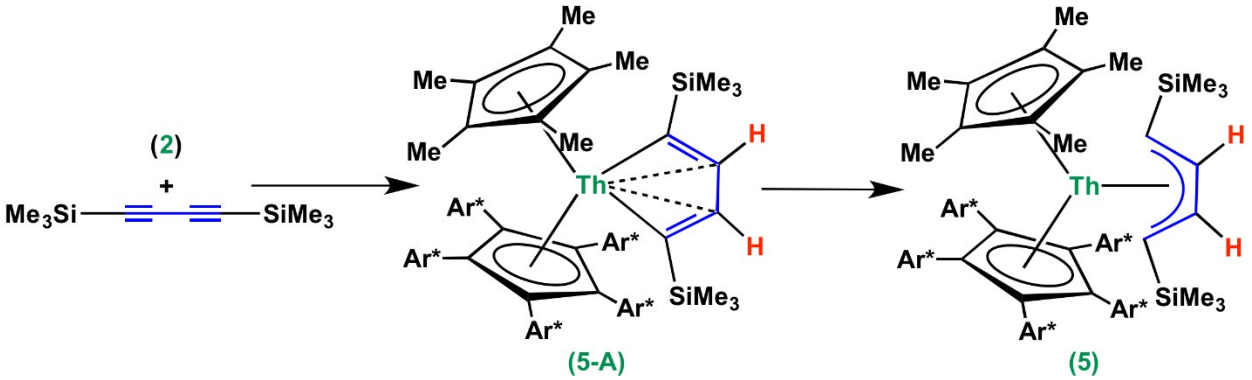
In the golvebox, [($Cp^{Ar*}$)Th(*p*-$CH_2$-$C_6H_4$-Me)$_3$] (**1**) (775 mg, 0.5 mmol) and ($Cp^{Me4}$)H (61 mg, 0.5 mmol) in THF (5 mL) were charged into a glass tube in a medium-pressure autoclave with a magnetic stirring bar. The autoclave was transferred outside of the glovebox and pressurized with $H_2$ to 20 atm. The mixture was stirred at room temperature for 12 h. Pressure was released and the autoclave was quickly returned to the glovebox. After filtration, all the volatiles were removed under vacuum. The residue was washed with cold hexane (1 mL) and dried under vacuum to give **3** (670 mg, 0.467 mmol, 93% yield) as a white solid. $^1$H NMR (500 MHz, $C_6D_6$): $\delta$ = 22.37 (s, 2H, Th-*H*), 7.35 (s, 10H, $C_5Ar_5$), 7.27 (s, 5H, $C_5Ar_5$), 6.01 (s, 1H, $C_5H$Me$_4$), 3.94~3.88 (m, 4H, *THF*), 2.55 (s, 6H, $C_5Me_4$), 2.52 (s, 6H, $C_5Me_4$), 1.44~1.38 (m, 4H, *THF*), 1.18 (s, 90H, Ar-$^t$*Bu*). $^{13}$C{$^1$H} NMR (126 MHz, $C_6D_6$): $\delta$ = 149.82 ($C_5Ar_5$), 135.98 ($C_5Ar_5$), 133.61 ($C_5$Ar$_5$), 127.78 ($C_5Ar_5$), 127.62 ($C_5Ar_5$), 126.06 ($C_5$Me$_4$), 119.91 ($C_5Ar_5$), 115.74 ($C_5$Me$_4$), 74.00 (*THF*), 35.05 ($C$(CH$_3$)$_3$), 31.91 (C($C$H$_3$)$_3$), 30.42 ($C_5$Me$_4$), 26.80 (*THF*), 14.52 ($C_5Me_4$), 13.00 ($C_5Me_4$). FT-IR (KBr, $cm^{-1}$): 3707, 3065, 2964, 2904, 2868, 1742, 1592, 1477, 1393, 1362, 1287, 1248, 1202, 1116, 1069, 933, 910, 899, 875, 713. Anal. calcd. for (**3**) $C_{88}H_{128}O_1Th_1$ (1434.00): C, 73.71; H, 9.00; found: C, 74.38; H, 9.35.

**Synthesis of [(Cp$^{Ar*}$)(Cp$^{*}$)Th(PhCH-C≡C-CHPh)] (4).**



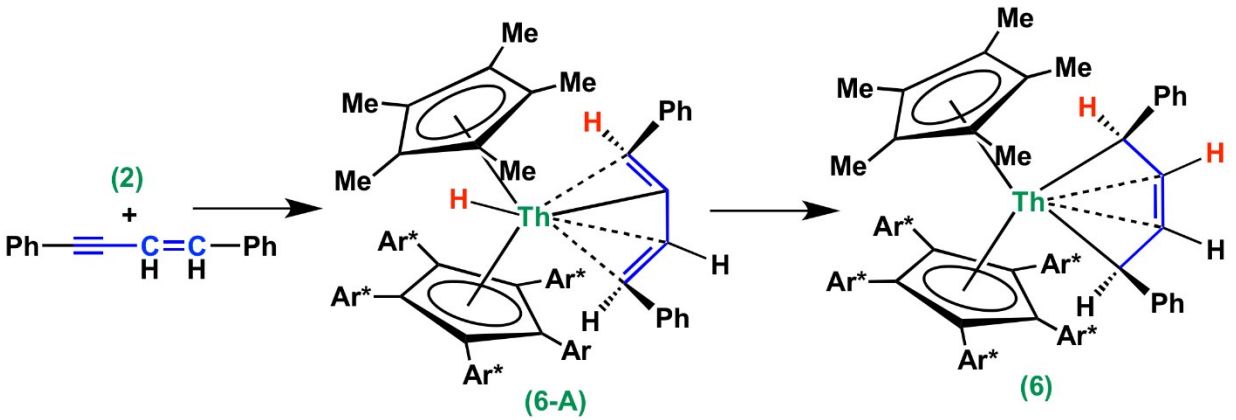

Solid 1,4-diphenyl-1,3-butadiyne (PhC≡C–C≡CPh) (14 mg, 0.069 mmol) was added in one portion to the hexane solution (5 mL) of [(Cp$^{Ar*}$)(Cp$^{*}$)ThH$_2$(THF)] (**2**) (100 mg, 0.069 mmol) at room temperature. The red brown mixture was stirred for 30 minutes at room temperature. After filtration, the solution was concentrated to 1 mL and kept at -30 $^{o}$C to give **4** (100 mg, 0.064 mmol, 93% yield) as red orange crystals. Single crystals of **4** · (1x$C_7H_8$ + 1.5x$C_6H_{14}$) suitable for X-ray analysis, were grown from hexane and toluene (10/1) at -30 $^{o}$C. $^{1}$H NMR (500 MHz, $C_6D_6$): $\delta$ = 7.36~7.31 (m, 8H, $C_6H_5$), 7.26 (t, $J$ = 7.5 Hz, 5H, $C_5Ar_5$), 7.09 (s, 10H, $C_5Ar_5$), 6.95 (t, $J$ = 7.4 Hz, 2H, $C_6H_5$), 4.88 (s, 2H, Ph-*CH*), 1.80 (s, 15H, $C_5Me_5$), 1.18 (s, 90H, Ar-$^{t}$*Bu*). $^{13}$C{1H} NMR (126 MHz, $C_6D_6$): $\delta$ = 150.39 ($C_5Ar_5$), 149.43 ($C_6H_5$), 143.56 ($C_5Ar_5$), 135.92 ($C_5Ar_5$), 132.98 ($C_6H_5$), 129.51 ($C_6H_5$), 128.74 ($C_6H_5$), 127.13 ($C_5Ar_5$), 126.98 ($C_6H_5$), 126.12 (PhCH-*C*≡*C*-CHPh), 125.87 ($C_5Me_5$), 123.38 (*Ph*CH-C≡C-CH*Ph*), 121.02 ($C_5Ar_5$&*Ph*CH-C≡C-CH*Ph*), 75.05 (PhCH-C≡C-*C*HPh), 35.13 ($C(CH_3)_3$), 31.90 (C($CH_3$)$_3$), 12.43 ($C_5Me_5$). FT-IR (KBr, cm$^{-1}$): 3657, 3064,3030, 2964, 2904, 2868, 1766, 1593, 1495, 1478, 1454, 1426, 1393, 1362, 1300, 1249, 1202, 1069, 1029, 936, 910, 899, 873, 776, 755, 728, 712, 695. Anal. calcd. for (**4**) $C_{101}H_{132}Th_1$ (1578.17): C, 76.87; H, 8.43; found: C, 77.23; H, 8.72.

**Synthesis of [(Cp$^{Ar*}$)(Cp*)Th(Me$_3$SiC⁼⁼CH⁼⁼CH⁼⁼C⁼⁼SiMe$_3$] (5).**




Solid 1,4-bistrimethylsilyl-1,3-butadiyne ($Me_3SiC{\equiv}C–C{\equiv}CSiMe_3$) (13.5 mg, 0.069 mmol) was added in one portion to the hexane solution (5 mL) of [($Cp^{Ar*}$)($Cp^*$)$ThH_2$(THF)] (**2**) (100 mg, 0.069 mmol) at room temperature. The red brown mixture was stirred for 12 h at room temperature and for 6h at 50 °C. After filtration, the solution was concentrated to 1 mL and kept at -30 °C to give **5** (51 mg, 0.032 mmol, 46% yield) as red orange crystals. Single crystals of **5** ·(1x$C_6H_{14}$) suitable for X-ray analysis, were grown from hexane at -30 °C. $^1$H NMR (500 MHz, $C_6D_6$): $\delta$ = 7.26 (s, 5H, $C_5Ar_5$), 7.07 (s, 10H, $C_5Ar_5$), 5.28~5.25 (m, 2H, $Me_3SiC$-*CH=CH*-$CSiMe_3$), 2.08 (s, 15H, $C_5Me_5$), 1.18 (s, 90H, Ar-$^t$*Bu*), 0.34 (s, 18H, $Me_3SiC$-CH=CH-$CSiMe_3$).$^{13}$C{$^1$H} NMR (126 MHz, $C_6D_6$): $\delta$ = 149.88 ($C_5Ar_5$), 138.55 ($C_5Ar_5$), 135.82 ($C_5Ar_5$), 127.47 ($C_5Ar_5$), 123.91 ($C_5Me_5$), 121.12 ($C_5Ar_5$), 120.76 ($Me_3SiC{\equiv}CH{\equiv}CH{\equiv}C{\equiv}SiMe_3$), 79.37 ($Me_3SiC{\equiv}CH{\equiv}CH{\equiv}C{\equiv}SiMe_3$), 35.10 ($C(CH_3)_3$), 32.07 ($C(CH_3)_3$), 13.33 ($C_5Me_5$), 4.55 ($Me_3SiC{\equiv}CH{\equiv}CH{\equiv}C{\equiv}SiMe_3$). FT-IR (KBr, cm$^{-1}$): 3662, 3064, 2963, 2904, 2868, 1780, 1692, 1478, 1392, 1362, 1300, 1248, 1202, 1152, 935, 924, 911, 898, 872, 863, 850, 839, 712. Anal. calcd. for (**5**) $C_{95}H_{140}Si_2Th_1$ (1570.34): C, 72.66; H, 8.97; found: C, 72.01; H, 9.33.

**Synthesis of [($Cp^{Ar*}$)($Cp^*$)Th(PhCH-CH=CH-CHPh)] (6).**



Solid (*E*)-1,4-diphenylbut-1-en-3-yne (PhC≡C–CH=CHPh) (14 mg, 0.069 mmol) was added in one portion to the hexane solution (5 mL) of [($Cp^{Ar*}$)($Cp^{*}$)$ThH_2$(THF)] (**2**) (100 mg, 0.069 mmol) at room temperature. The red brown mixture was stirred for 30 minutes at room temperature. After filtration, the solution was concentrated to 1 mL and kept at -30 °C to give **6** (102 mg, 0.066 mmol, 95% yield) as yellow orange crystals. Single crystals of **6** · (2x$C_6H_{14}$) suitable for X-ray analysis, were grown from hexane at -30 °C. $^1$H NMR (500 MHz, $C_6D_6$) $\delta$ = 7.29 (m, 5H, $C_5$*Ar*$_5$), 7.20 (m, 7H, *Ph*), 7.16 (m, 11H, $C_5$*Ar*$_5$*&Ph*), 7.03~6.92 (m, 2H, *Ph*), 5.70~5.59 (m, 2H, CH-C*H*=C*H*-CH), 2.42~2.29 (m, 2H, C*H*-CH=CH-C*H*), 1.94 (s, 15H, $C_5$*Me*$_5$), 1.09 (s, 90H, Ar-$^t$*Bu*). $^{13}$C{$^1$H} NMR (126 MHz, $C_6D_6$): $\delta$ = 150.36 ($C_5$*Ar*$_5$), 147.11(*Ph*CH-CH=CH-CH*Ph*), 136.86 ($C_5$*Ar*$_5$), 133.94 (*C*$_5$Ar$_5$), 128.75 (*Ph*CH-CH=CH-CH*Ph*), 128.53 (*Ph*CH-CH=CH-CH*Ph*), 127.70 ($C_5$*Ar*$_5$), 123.58 (*Ph*CH-CH=CH-CH*Ph*), 123.34 (*C*$_5$Me$_5$), 120.93 ($C_5$*Ar*$_5$), 113.37 (PhCH-*C*H=*C*H-CHPh), 95.41(Ph*C*H-CH=CH-*C*HPh), 35.01(*C*($CH_3$)$_3$), 31.80 (C(*C*$H_3$)$_3$), 12.99 ($C_5$*Me*$_5$). FT-IR (KBr, cm$^{-1}$): 3658, 3063, 3027, 2963, 2904, 2867, 1786, 1593, 1494, 1393, 1362, 1302, 1249, 1202, 1080, 1030, 969, 934, 923, 910, 899, 874, 740, 712, 699. Anal. calcd. for (**6**) $C_{101}H_{134}Th_1$ (1580.18): C, 76.77; H, 8.55; found: C, 77.33; H, 8.86.

**Synthesis of [($Cp^{Ar*}$)($Cp^{*}$)ThH(PhC=CHPh)] (7).**

Solid diphenylacetylene (PhC≡CPh) (12.3 mg, 0.069 mmol) was added in one portion to the hexane solution (5 mL) of [($Cp^{Ar*}$)($Cp^{*}$)$ThH_2$(THF)] (**2**) (100 mg, 0.069 mmol) at room temperature. The yellow brown mixture was stirred for 12 h at room temperature. After filtration, the solution was concetrated to 1 mL and ketp at -30 °C to give **7** (96 mg, 0.062 mmol, 90% yield) as pale-yellow crystals. Single crystals of **7** · (1x$C_7H_8$ **+** 2x$C_6H_{14}$) suitable for X-ray analysis, were grown from hexane and toluene (10/1) at -30 °C. $^1$H NMR (500 MHz, $C_6D_6$): $\delta$ = 15.73 (s, 1H, Th-*H*), 7.82 (d, *J* = 7.6 Hz, 2H, *Ph*), 7.29 (d, *J* = 2.0 Hz, 6H, $C_5$*Ar*$_5$*&Ph*), 7.25 (s, 8H, $C_5$*Ar*$_5$), 7.13~6.93 (m, 5H, $C_5$*Ar*$_5$*&Ph*), 6.61 (dd, *J* = 9.5, 5.2 Hz, 3H, *Ph&Ph-CH*), 2.24 (s, 15H, $C_5$*Me*$_5$), 1.13 (s, 90H, Ar-$^t$*Bu*). $^{13}$C{$^1$H} NMR (126 MHz, $C_6D_6$): $\delta$ = 218.14 (Ph*C*=CHPh), 150.16 ($C_5$*Ar*$_5$), 145.45 (*Ph*C=CH*Ph*), 136.23 ($C_5$*Ar*$_5$), 133.90 (*Ph*C=CH*Ph*), 132.47 (*Ph*C=CH*Ph*), 130.27 (*C*$_5$Ar$_5$), 128.65 (*Ph*C=CH*Ph*), 128.53 (*Ph*C=CH*Ph*), 127.30 ($C_5$*Ar*$_5$), 127.23 ($C_5$*Ar*$_5$), 125.23 (*C*$_5$Me$_5$), 125.12 (*Ph*C=CH*Ph*), 120.81 (*Ph*C=CH*Ph*), 108.87 (PhC=*C*HPh), 35.01 (*C*($CH_3$)$_3$), 31.90 (C(*C*$H_3$)$_3$), 13.40 ($C_5$*Me*$_5$). FT-IR (KBr, cm$^{-1}$): 3659, 3061,

2964, 2904, 2868, 1767, 1592, 1477, 1393, 1362, 1300, 1249, 1202, 1076, 1028, 923, 911, 898, 874, 780, 756, 712, 699. Anal. calcd. for (**7**) $C_{99}H_{132}Th_1$ (1554.14): C, 76.51; H, 8.56; found: C, 76.92; H, 9.00.

## 2. Selected NMR Spectra

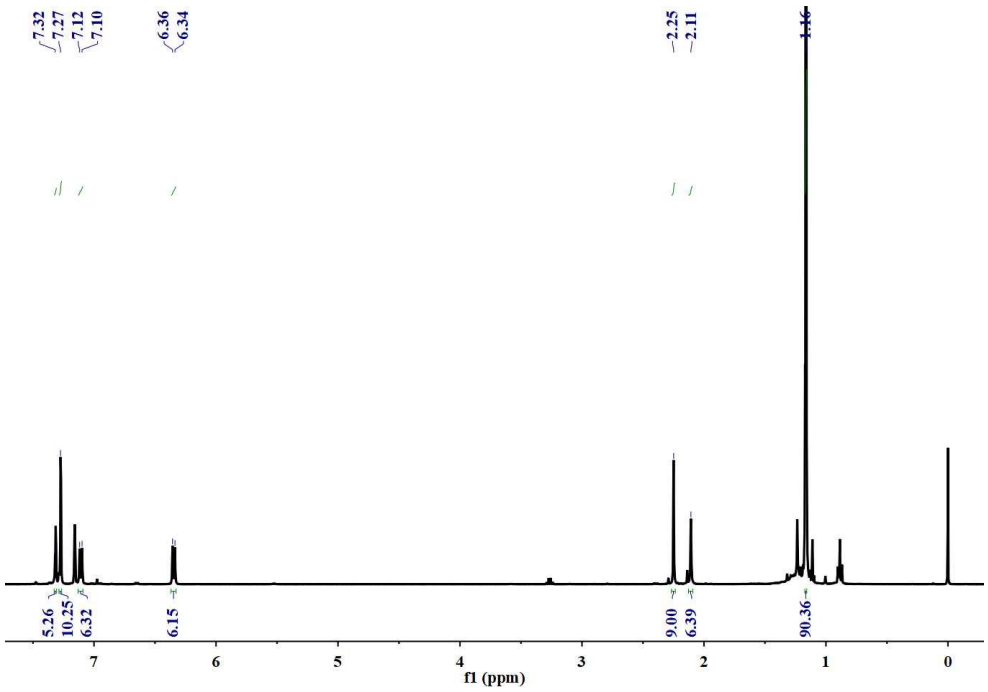



**Figure S1.** $^{1}H$ NMR spectrum (400 MHz) of complex **1** in $C_6D_6$ at 25 °C.

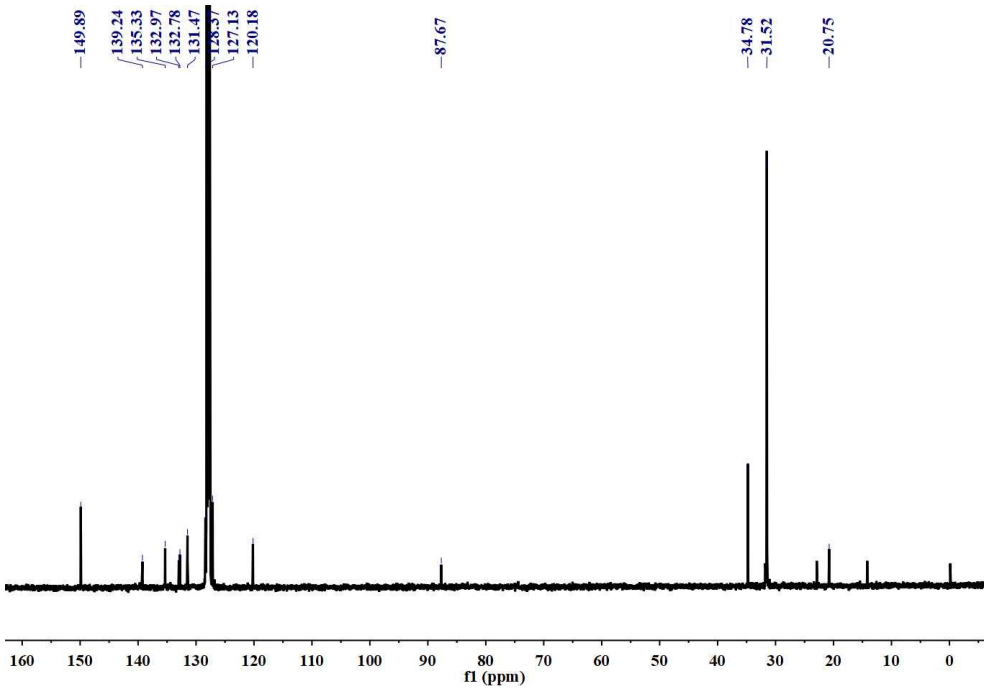



**Figure S2.** $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz) of complex **1** in $C_6D_6$ at 25 °C.

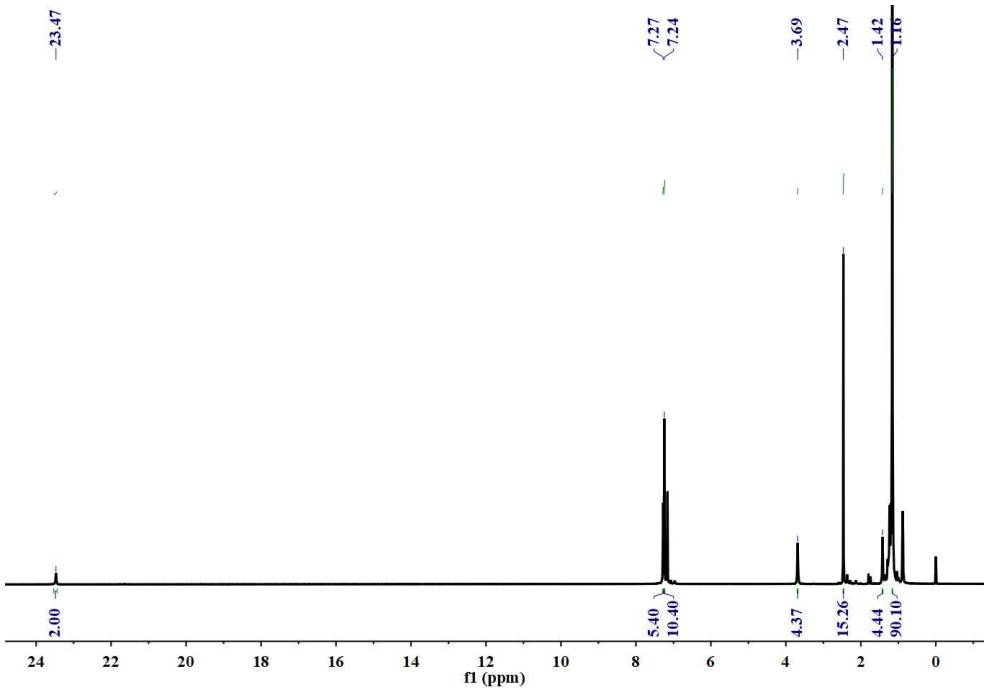



**Figure S3.** $^{1}H$ NMR spectrum (500 MHz) of complex **2** in $C_6D_6$ at 25 °C.

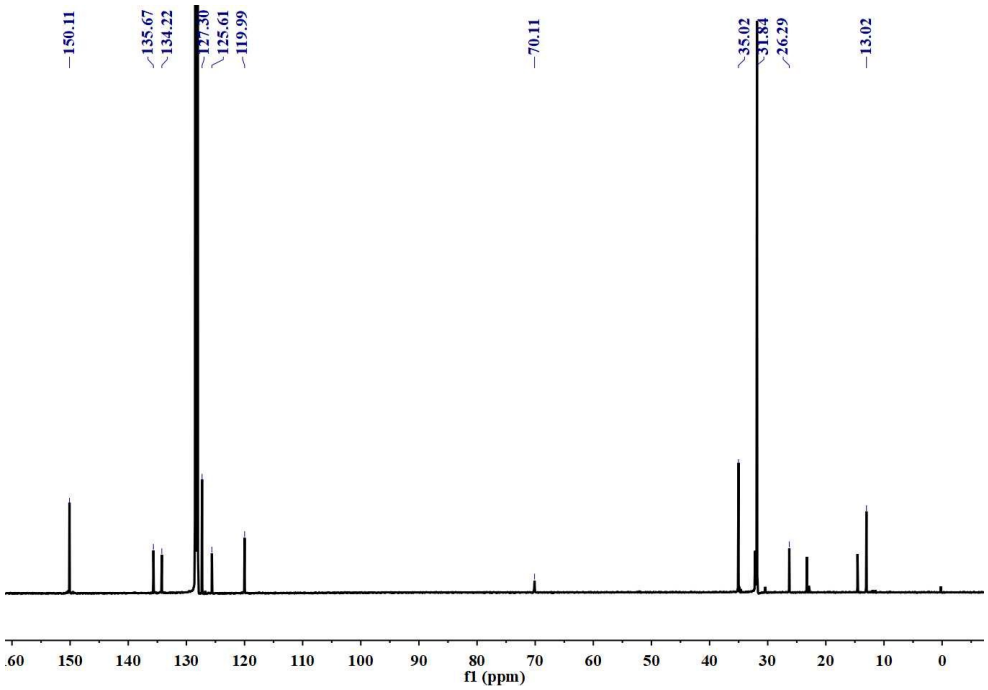



**Figure S4.** $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz) of complex **2** in $C_6D_6$ at 25 °C.

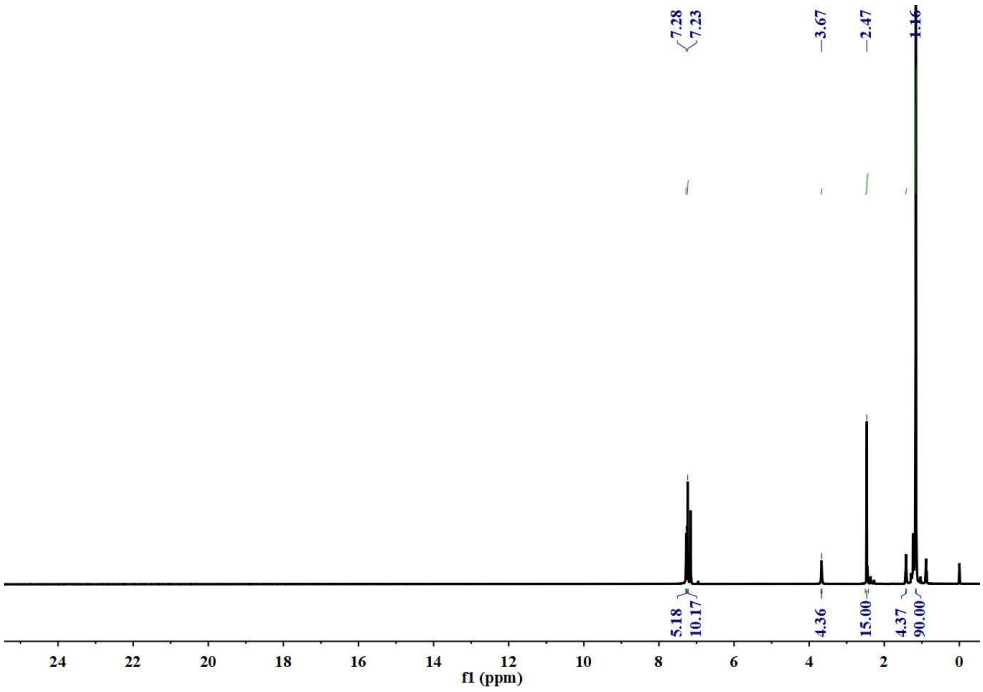



**Figure S5.** $^{1}H$ NMR spectrum (500 MHz) of complex **2-D** in $C_6D_6$ at 25 $^{o}C$.

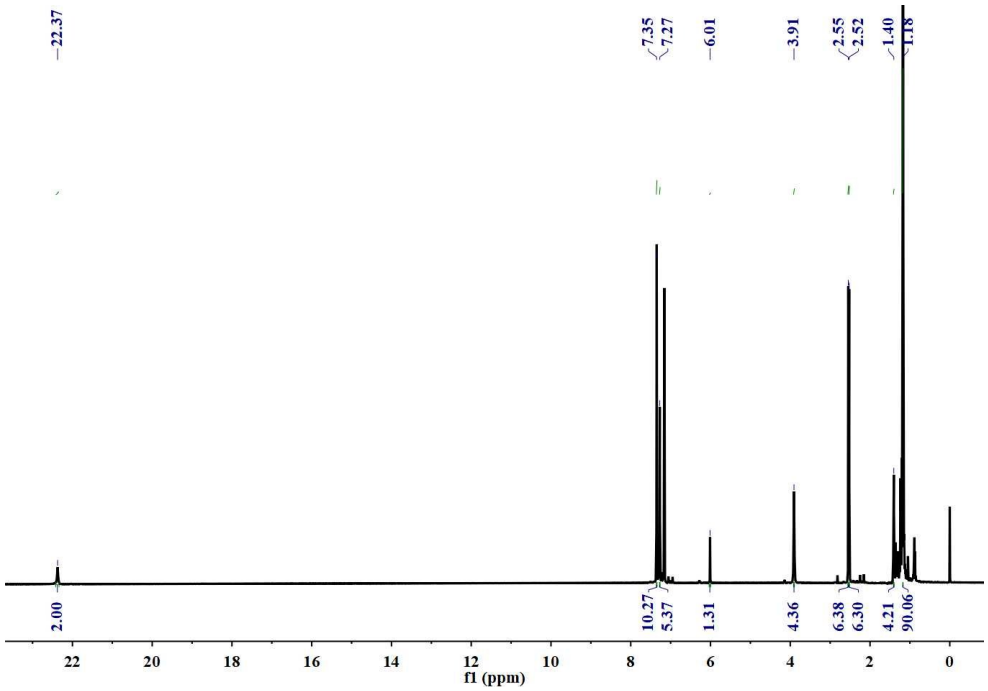



**Figure S6.** $^{1}H$ NMR spectrum (500 MHz) of complex **3** in $C_6D_6$ at 25 °C.

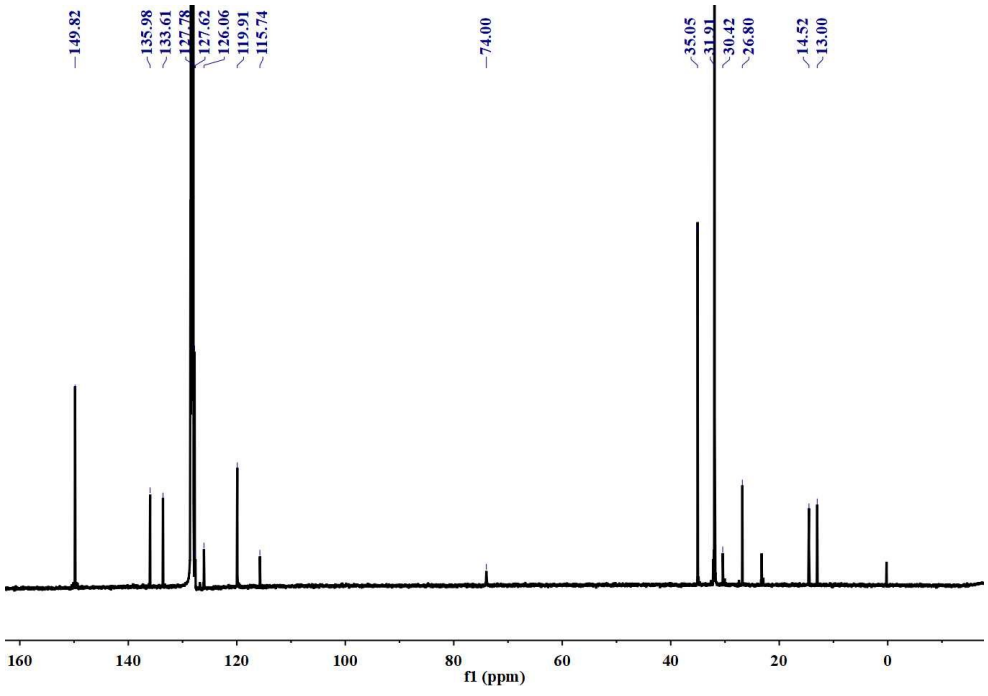



**Figure S7.** $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz) of complex **3** in $C_6D_6$ at 25 °C.

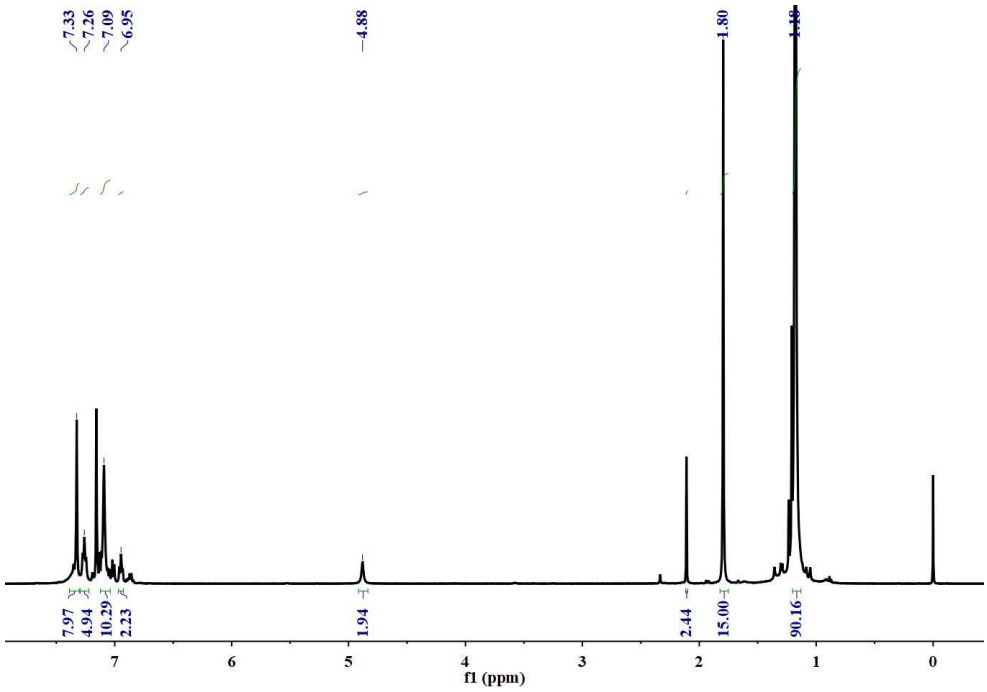



**Figure S8.** $^{1}H$ NMR spectrum (500 MHz) of complex **4** in $C_6D_6$ at 25 °C.

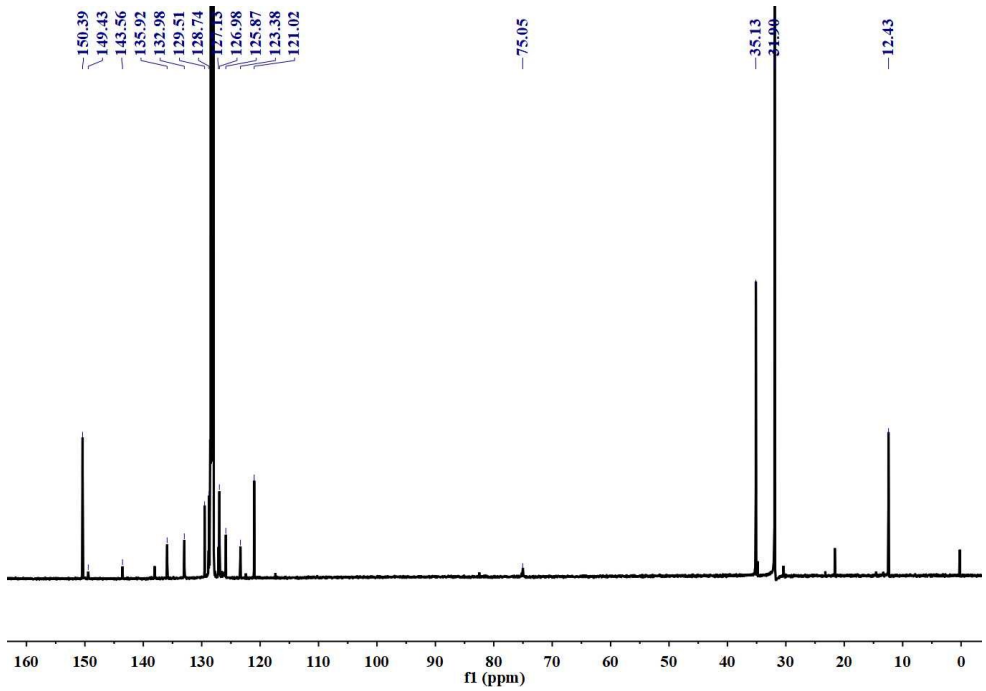



**Figure S9.** $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz) of complex **4** in $C_6D_6$ at 25 °C.

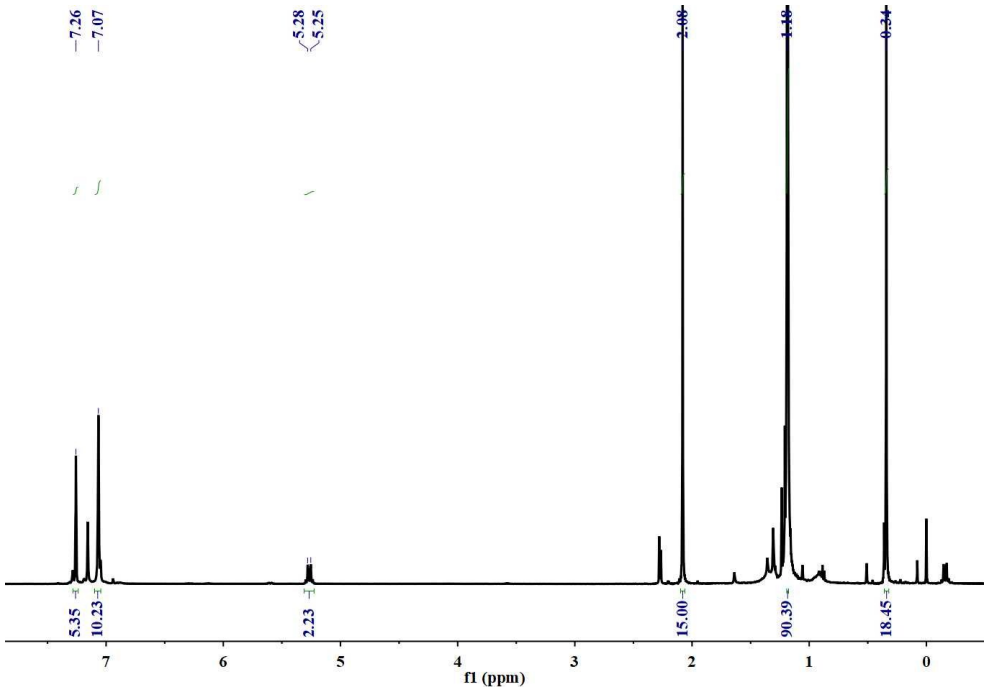



**Figure S10.** $^{1}H$ NMR spectrum (500 MHz) of complex **5** in $C_6D_6$ at 25 °C.

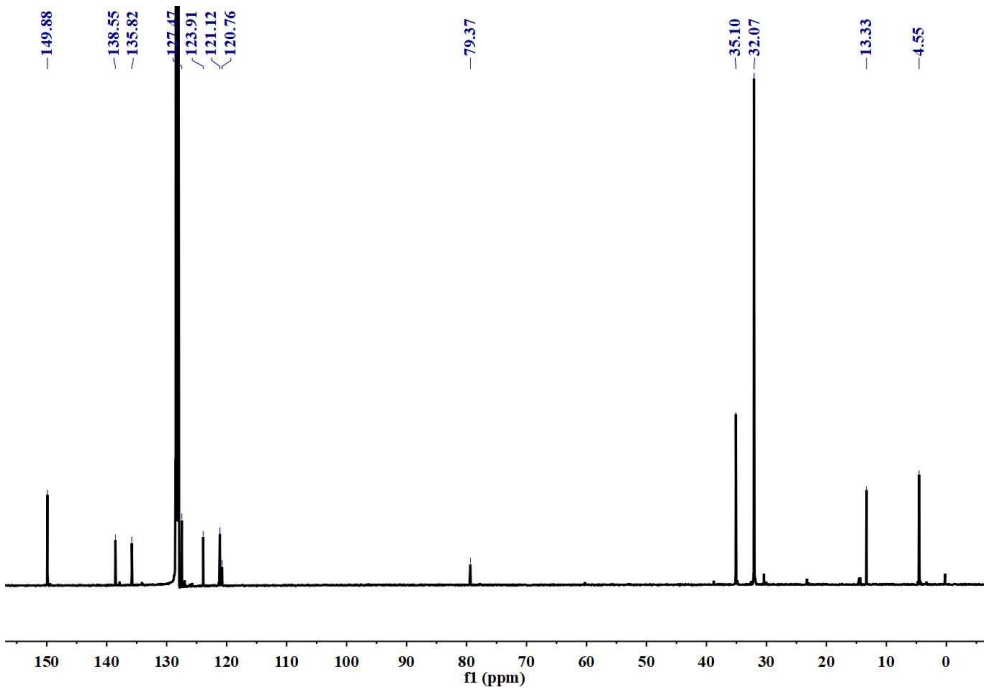



**Figure S11.** $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz) of complex **5** in $C_6D_6$ at 25 °C.

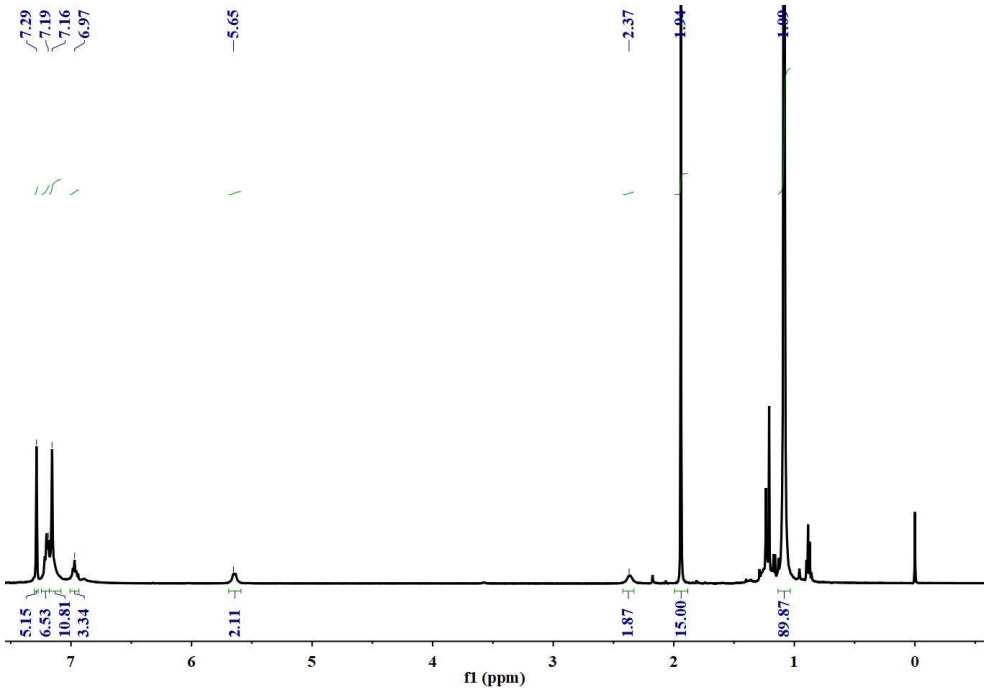



**Figure S12.** $^{1}$H NMR spectrum (500 MHz) of complex **6** in $C_6D_6$ at 25 $^{o}$C.

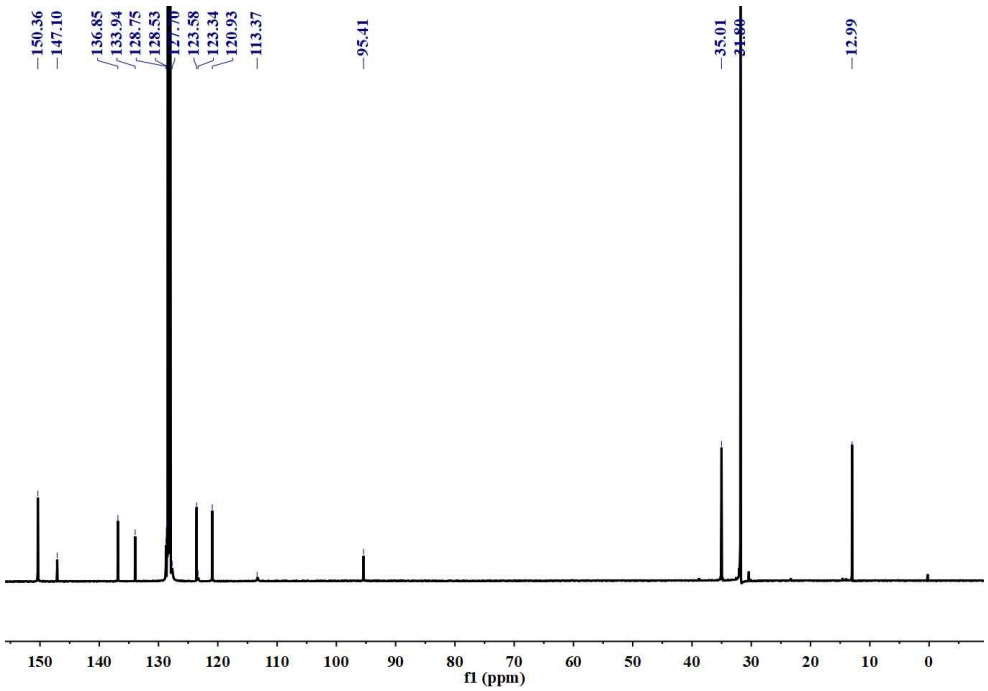



**Figure S13.** $^{13}$C{$^{1}$H} NMR spectrum (126 MHz) of complex **6** in $C_6D_6$ at 25 $^{o}$C.

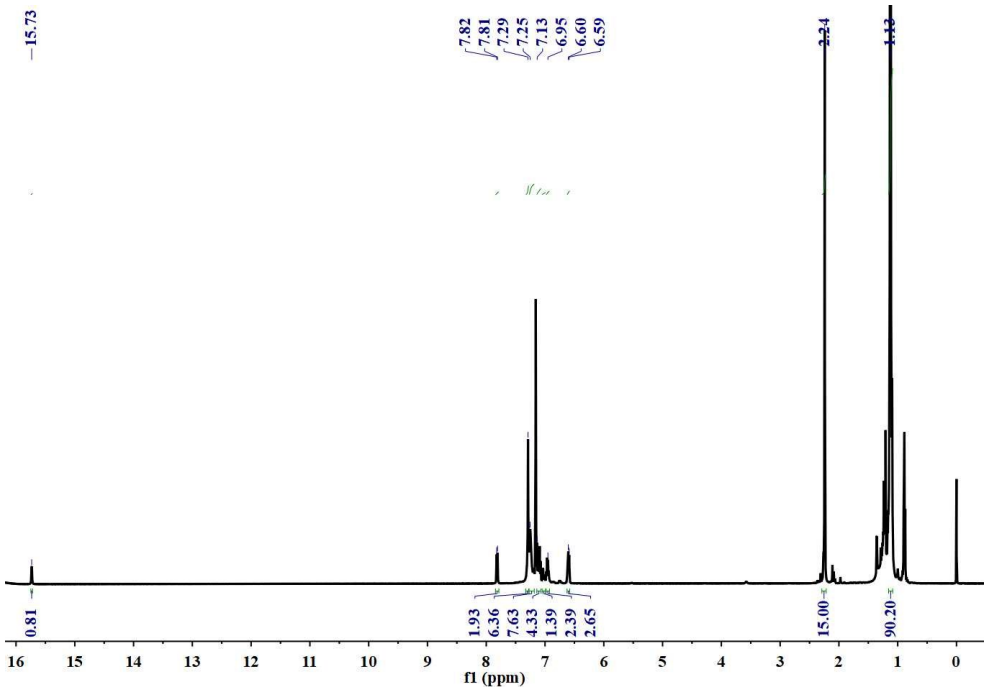



**Figure S14.** $^{1}H$ NMR spectrum (500 MHz) of complex **7** in $C_6D_6$ at 25 °C.

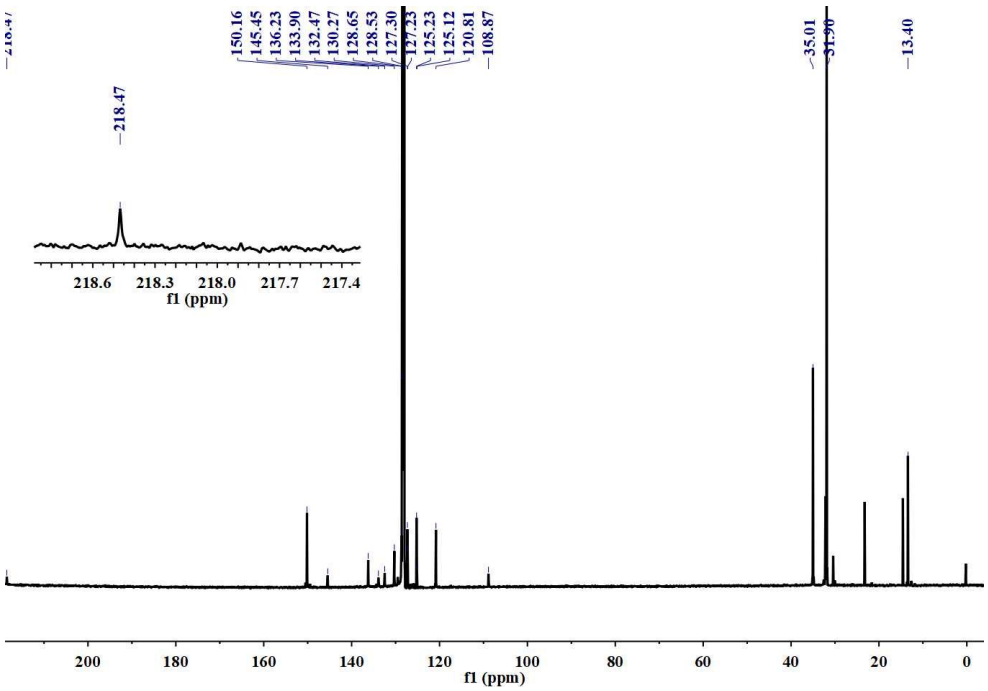



**Figure S15.** $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz) of complex **7** in $C_6D_6$ at 25 °C.

## 3. X-ray Crystallographic Studies

Single crystals suitable for X-Ray analysis were obtained as described in the preparation. The crystals were manipulated under a microscope in the glovebox, Data collection was performed at -80 °C on a Bruker SMART APEX diffractrometer with a CCD area detector, using graphite monochromated Mo $K_\alpha$ radiation ($\lambda$ = 0.71073 Å). The determination of the crystal class and unit cell parameters was carried out by the SMART program packages.[5] The raw frame data were processed using SAINT[6] and absorption corrections using SADABS[7] to yield the reflection data file. The structures were solved by using SHELXS-2018,[8] SIR-97[9] or SUPERFLIP[10] in the WINGX program package.[11] Refinements were performed on $F^2$ anisotropically for all the non-hydrogen atoms by the full-matrix least-squares method using SHELXL-2018 program.[8]

Refinement of **1**: The SQUEEZE[12] routine of the program PLATON[13] was implemented to remove the contributions of two disordered hexanes to the observed structure factors. Three $^t$Bu groups in the $Cp^{Ar*}$ ligand were disordered. C40~C42 and C40'~C42' disordered over two sites with occupancies 0.245:0.755. C96~C98 and C96'~C98' disordered over two sites with occupancies 0.552:0.448. C102~C104 and C202~C204 disordered over two sites with occupancies 0.488:0.512.

Refinement of **2**: The SQUEEZE[12] routine of the program PLATON[13] was implemented to remove the contributions of 1.5 disordered hexanes to the observed structure factors. The terminal hydrides (H1 and H2) were located by difference Fourier syntheses and refined. C71~C73 and C71'~C73' disordered over two sites with occupancies 0.496:0.504. The THF ligand (O1, C3~C6 and O1', C3'~C6') disordered over two sites with occupancies 0.512:0.488.

Refinement of **4**: The SQUEEZE[12] routine of the program PLATON[13] was implemented to remove the contributions of one disordered toluene and 1.5 disordered hexanes to the observed structure factors. The hydrogen atoms (H1 and H4) in the PhCH-C≡C-CHPh unit were located by difference Fourier syntheses and refined isotropically. Two $^t$Bu groups in the $Cp^{Ar*}$ ligand were disordered. C73~C75 and C73'~C75' disordered over two sites with occupancies 0.578:0.422. C87~C89 and C87'~C89' disordered over two sites with occupancies 0.728:0.272.

Refinement of **5**: The SQUEEZE[12] routine of the program PLATON[13] was implemented to remove the contributions of the disordered hexane to the observed structure factors. The

hydrogen atoms (H2 and H3) in the $Me_3SiC$-CH=CH-$CSiMe_3$ unit were located by difference Fourier syntheses, and refined isotropically. Three $^t$Bu groups in the $Cp^{Ar*}$ ligand were disordered. C44~C46 and C44'~C46' disordered over two sites with occupancies 0.504:0.496. C50~C52 and C50'~C52' disordered over two sites with occupancies 0.576:0.424. C58~C60, and C58'~C60' disordered over two sites with occupancies 0.592:0.408.

Refinement of **6**: The SQUEEZE[12] routine of the program PLATON[13] was implemented to remove the contributions of the two disordered hexanes to the observed structure factors. The hydrogen atoms (H1, H2, H3 and H4) of PhCH-CH=CH-CHPh unit were located by difference Fourier syntheses and refined isotropically. Two $^t$Bu groups in the $Cp^{Ar*}$ ligand were disordered. C45~C47 and C45'~C47' disordered over two sites with occupancies 0.322:0.678. C87~C89 and C87'~C89' disordered over two sites with occupancies 0.708:0.292.

Refinement of **7**: The SQUEEZE[12] routine of the program PLATON[13] was implemented to remove the contributions of the disordered solvents (one toluene and two hexanes) to the observed structure factors. The terminal hydride (H1) and the hydrogen atom (H3) of PhC-=CHPh unit were located by difference Fourier syntheses, and refined isotropically. Three $^t$Bu groups in the $Cp^{Ar*}$ ligand were disordered. C39~C41 and C39'~C41' disordered over two sites with occupancies 0.641:0.359. C81~C83 and C81'~C83' disordered over two sites with occupancies 0.693:0.307. C87~C89 and C87'~C89' disordered over two sites with occupancies 0.725:0.275.

Other hydrogen atoms were placed at the calculated positions and were included in the structure calculation without further refinement of the parameters. The residual electron densities were of no chemical significance. Crystal data and analysis results are listed in STable **1-6**.

CCDC number 1877537 (**1**), 1877538 (**2**), 1877539 (**4**), 1877540 (**5**), 1877541 (**6**) and 1877542 (**7**) contain the supplementary crystallographic data for this paper. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+44)1223-336-033; E-mail: deposit@ccdc.cam.ac.uk).

**Table S1.** Crystal data and structure refinement for Complex **1.**

| | |
|---|---|
| Identification code | D033 |
| Empirical formula | $C_{99}H_{132}Th_1$ •(2 x Hexane) |
| Formula weight | 1554.08 |
| Temperature | 193(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Monoclinic, C2/c |
| a | 25.9020(5) Å |
| b | 16.9604(3) Å |
| c | 47.2064(9) Å |
| α | 90 ° |
| β | 104.1160(10) ° |
| γ | 90 ° |
| Volume | 20111.9(7) $Å^3$ |
| Z, Calculated density | 8, 1.026 $Mg/m^3$ |
| Absorption coefficient | 1.520 $mm^{-1}$ |
| F(000) | 6528 |
| Crystal size | 0.280 x 0.250 x 0.200 mm |
| Theta range for data collection | 1.456 to 24.998 ° |
| Limiting indices | -28<=h<=30, -20<=k<=20, -55<=l<=53 |
| Reflections collected / unique | 62628 / 17013 [R(int) = 0.0655] |
| Completeness to theta | (24.998 °) 96.0 % |
| Absorption correction | Empirical |
| Max. and min. transmission | 0.738 and 0.660 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 17013 / 48 / 805 |
| Goodness-of-fit on $F^2$ | 1.002 |
| Final R indices [I>2sigma(I)] | R1 = 0.0518, wR2 = 0.1245 |
| R indices (all data) | R1 = 0.0840, wR2 = 0.1397 |
| Largest diff. peak and hole | 1.685 and -1.024 e. $Å^{-3}$ |

**Table S2.** Crystal data and structure refinement for Complex **2.**

| | |
|---|---|
| Identification code | D082 |
| Empirical formula | $C_{89}H_{130}O_1Th_1$ •(1.5 x Hexane) |
| Formula weight | 1447.96 |
| Temperature | 193(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Triclinic, P-1 |
| a | 14.7237(17) Å |
| b | 14.9064(17) Å |
| c | 24.091(3) Å |
| α | 97.141(3) ° |
| β | 95.688(2) ° |
| γ | 118.572(3) ° |
| Volume | 4530.7(9) $Å^3$ |
| Z, Calculated density | 2, 1.061 $Mg/m^3$ |
| Absorption coefficient | 1.684 $mm^{-1}$ |
| F(000) | 1524 |
| Crystal size | 0.190 x 0.170 x 0.120 mm |
| Theta range for data collection | 2.135 to 25.000 ° |
| Limiting indices | -17<=h<=17, -17<=k<=17, -16<=l<=28 |
| Reflections collected / unique | 23279 / 15513 [R(int) = 0.1487] |
| Completeness to theta | (25.00 °) 97.3 % |
| Absorption correction | Empirical |
| Max. and min. transmission | 0.817 and 0.733 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 15513 / 39 / 505 |
| Goodness-of-fit on $F^2$ | 0.871 |
| Final R indices [I>2sigma(I)] | R1 = 0.0941, wR2 = 0.1562 |
| R indices (all data) | R1 = 0.2170, wR2 = 0.1994 |

| | |
|---|---|
| Largest diff. peak and hole | 1.126 and -1.380 e. $Å^{-3}$ |

**Table S3.** Crystal data and structure refinement for Complex **4.**

| | |
|---|---|
| Identification code | D133 |
| Empirical formula | $C_{101}H_{132}Th_1$•(1.5 x Hexane + Toluene) |
| Formula weight | 1578.10 |
| Temperature | 193(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Triclinic, P-1 |
| a | 14.7678(11) Å |
| b | 15.0111(11) Å |
| c | 23.5344(17) Å |
| α | 108.0040(10) ° |
| β | 90.7910(10) ° |
| γ | 91.2300(10) ° |
| Volume | 4959.4(6) $Å^3$ |
| Z, Calculated density | 2, 1.057 $Mg/m^3$ |
| Absorption coefficient | 1.542 $mm^{-1}$ |
| F(000) | 1656 |
| Crystal size | 0.280 x 0.240 x 0.220 mm |
| Theta range for data collection | 1.636 to 25.000 ° |
| Limiting indices | -17<=h<=17, -17<=k<=9, -26<=l<=27 |
| Reflections collected / unique | 24993 / 16957 [R(int) = 0.0271] |
| Completeness to theta | (25.00 °) 97.0 % |
| Absorption correction | Empirical |
| Max. and min. transmission | 0.712 and 0.656 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 16957 / 30 / 948 |
| Goodness-of-fit on $F^2$ | 1.007 |
| Final R indices [I>2sigma(I)] | R1 = 0.0381, wR2 = 0.0854 |
| R indices (all data) | R1 = 0.0489, wR2 = 0.0917 |
| Largest diff. peak and hole | 1.218 and -0.519 e. $Å^{-3}$ |

**Table S4.** Crystal data and structure refinement for Complex **5.**

| | |
|---|---|
| Identification code | D138 |
| Empirical formula | $C_{95}H_{140}Si_2Th_1$•(Hexane) |
| Formula weight | 1570.28 |
| Temperature | 193(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Monoclinic, P2(1)/c |
| a | 15.5087(8) Å |
| b | 20.6680(11) Å |
| c | 30.4806(16) Å |
| α | 90 ° |
| β | 101.2300(10) ° |
| γ | 90 ° |
| Volume | 9583.0(9) $Å^3$ |
| Z, Calculated density | 4, 1.088 $Mg/m^3$ |
| Absorption coefficient | 1.620 $mm^{-1}$ |
| F(000) | 3312 |
| Crystal size | 0.280 x 0.200 x 0.150 mm |
| Theta range for data collection | 1.662 to 24.999 ° |
| Limiting indices | -18<=h<=13, -24<=k<=23, -36<=l<=31 |
| Reflections collected / unique | 49096 / 16759 [R(int) = 0.0983] |
| Completeness to theta | (24.999 °) 99.2 % |
| Absorption correction | Empirical |
| Max. and min. transmission | 0.784 and 0.685 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 16759 / 46 / 829 |
| Goodness-of-fit on $F^2$ | 0.934 |
| Final R indices [I>2sigma(I)] | R1 = 0.0466, wR2 = 0.1057 |
| R indices (all data) | R1 = 0.0721, wR2 = 0.1156 |
| Largest diff. peak and hole | 1.916 and -1.052 e. $Å^{-3}$ |

**Table S5.** Crystal data and structure refinement for Complex **6.**

| | |
|---|---|
| Identification code | D199 |
| Empirical formula | $C_{101}H_{134}Th_1$•(2 x Hexane) |
| Formula weight | 1580.11 |
| Temperature | 193(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Monoclinic, P2(1)/n |
| a | 15.7332(10) Å |
| b | 39.615(3) Å |
| c | 16.3475(10) Å |
| α | 90 ° |
| β | 98.6040(10) ° |
| γ | 90 ° |
| Volume | 10074.1(11) $Å^3$ |
| Z, Calculated density | 4, 1.042 $Mg/m^3$ |
| Absorption coefficient | 1.519 $mm^{-1}$ |
| F(000) | 3320 |
| Crystal size | 0.240 x 0.190 x 0.140 mm |
| Theta range for data collection | 1.665 to 26.437 ° |
| Limiting indices | -17<=h<=19, -49<=k<=49, -20<=l<=14 |
| Reflections collected / unique | 47917 / 18733 [R(int) = 0.0861] |
| Completeness to theta | (25.242 °) 89.6 % |
| Absorption correction | Empirical |
| Max. and min. transmission | 0.808 and 0.714 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 18733 / 34 / 900 |
| Goodness-of-fit on $F^2$ | 0.716 |
| Final R indices [I>2sigma(I)] | R1 = 0.0468, wR2 = 0.0805 |
| R indices (all data) | R1 = 0.0971, wR2 = 0.0897 |
| Largest diff. peak and hole | 1.075 and -0.737 e. $Å^{-3}$ |

**Table S6.** Crystal data and structure refinement for Complex **7.**

| | |
|---|---|
| Identification code | D156 |
| Empirical formula | $C_{99}H_{132}Th_1$•(2 x Hexane + Toluene) |
| Formula weight | 1554.08 |
| Temperature | 193(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Triclinic, P-1 |
| a | 13.7094(7) Å |
| b | 15.5474(8) Å |
| c | 24.9054(13) Å |
| α | 85.2590(10) ° |
| β | 80.1530(10) ° |
| γ | 72.0580(10) ° |
| Volume | 4973.4(4) $Å^3$ |
| Z, Calculated density | 2, 1.038 $Mg/m^3$ |
| Absorption coefficient | 1.537 $mm^{-1}$ |
| F(000) | 1632 |
| Crystal size | 0.200 x 0.170 x 0.110 mm |
| Theta range for data collection | 1.580 to 25.000 ° |
| Limiting indices | -16<=h<=9, -18<=k<=16, -29<=l<=27 |
| Reflections collected / unique | 25569 / 17122 [R(int) = 0.0324] |
| Completeness to theta | (25.00 °) 97.7 % |
| Absorption correction | Empirical |
| Max. and min. transmission | 0.844 and 0.743 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 17122 / 46 / 837 |
| Goodness-of-fit on $F^2$ | 1.009 |
| Final R indices [I>2sigma(I)] | R1 = 0.0472, wR2 = 0.1133 |
| R indices (all data) | R1 = 0.0594, wR2 = 0.1210 |
| Largest diff. peak and hole | 1.382 and -1.160 e. $Å^{-3}$ |

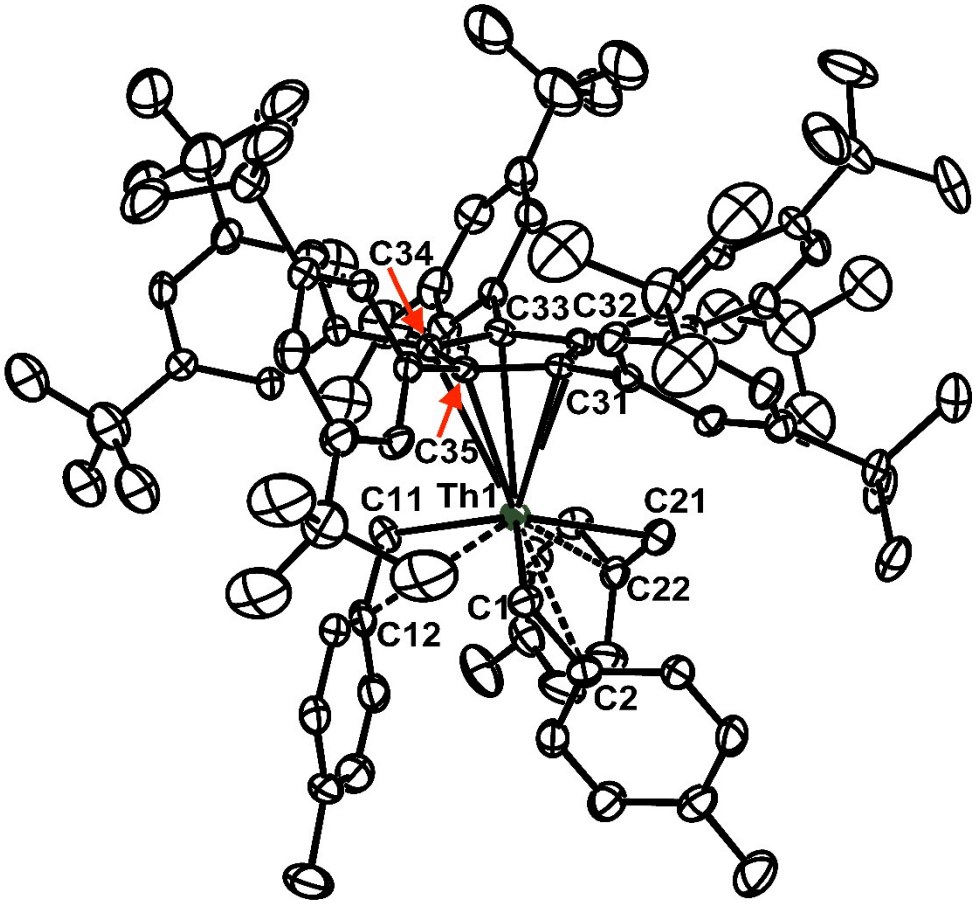



**Figure S16.** ORTEP plot (30% probability) of [($Cp^{Ar*}$)Th(*p*-$CH_2$-$C_6H_4$-$CH_3$)$_3$] (**1**). All the hydrogen atoms are omitted for clarity. Selected interatomic distances [Å]: Th1—C1 2.518(5), Th1—C2 3.023(5), Th1—C11 2.519(6), Th1—C12 3.006(5), Th1—C21 2.491(6), Th1—C22 2.898(6), Th1—C31 2.811(5), Th1—C32 2.857(5), Th1—C33 2.898(5), Th1—C34 2.915(5), Th1—C35 2.856(5), Th1—Cent1 2.598.

- Cent1: Centre of the $Cp^{Ar*}$ ring (C31~C35).

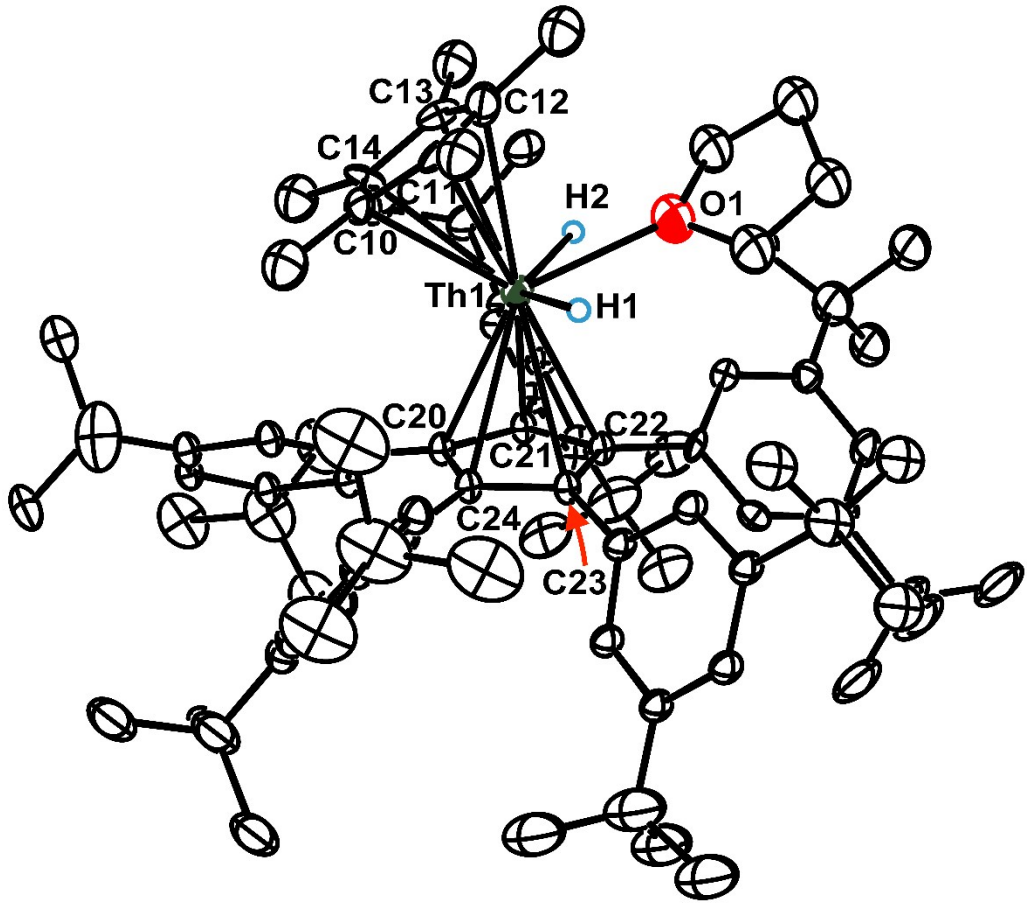



**Figure S17.** ORTEP plot (30% probability) of [($Cp^{Ar*}$)($Cp^{*}$)$ThH_2$(THF)] (**2**). All the hydrogen atoms, except the terminal hydrides (H1 and H2), are omitted for clarity. Selected interatomic distances [Å] and angles [deg]: Th1—H1 2.07(10), Th1—H2 2.20(10), Th1—O1 2.45(2), Th1—C10 2.750(11), Th1—C11 2.830(12), Th1—C12 2.794(16), Th1—C13 2.795(13), Th1—C14 2.727(12), Th1—C20 2.881(13), Th1—C21 2.880(12), Th1—C22 2.869(12), Th1—C23 2.888(12), Th1—C24 2.869(12), Th1—Cent1 2.608, Th1—Cent2 2.511, Cent1—Th1—Cent2 146.7, H1—Th1—H2 131(4).

- Cent1: Centre of the $Cp^{Ar*}$ ring (C31~C35);
- Cent2: Centre of the $Cp^{*}$ ring (C20~C24).

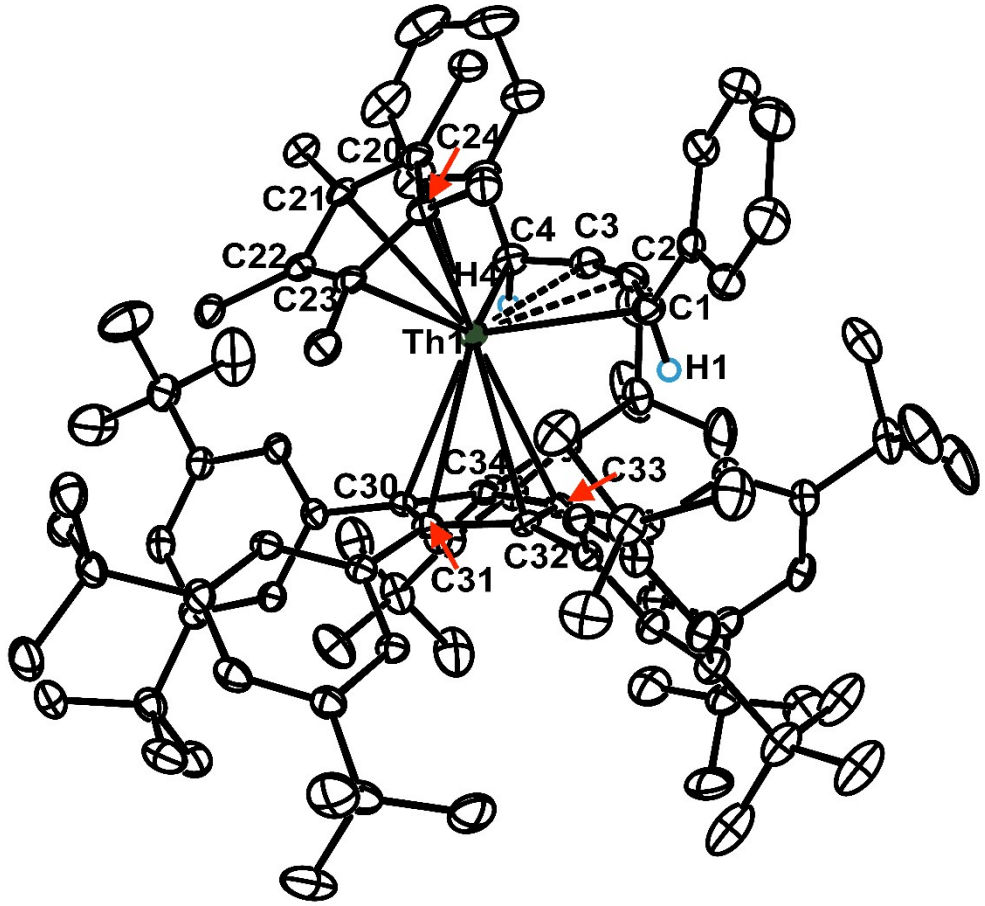



**Figure S18.** ORTEP plot (30% probability) of [($Cp^{Ar*}$)($Cp^{*}$)Th(PhCH-C≡C-CHPh)] (**4**). All the hydrogen atoms, except H1 and H4, are omitted for clarity. Selected interatomic distances [Å] and angles [deg]: C1—C2 1.423(6), C2—C3 1.238(6), C3—C4 1.404(6), Th1—C1 2.684(4), Th1—C2 2.528(4), Th1—C3 2.526(4), Th1—C4 2.666(4), Th1—C20 2.830(3), Th1—C21 2.802(3), Th1—C22 2.798(4), Th1—C23 2.802(4), Th1—C24 2.825(3), Th1—C30 2.906(3), Th1—C31 2.869(3), Th1—C32 2.877(3), Th1—C33 2.977(3), Th1—C34 2.978(3), Th1—Cent1 2.657, Th1—Cent2 2.539; C4—C3—C2 155.7(5), C3—C2—C1 156.0(4), Cent1—Th1—Cent2 138.23.

- Cent1: Centre of the $Cp^{Ar*}$ ring (C30~C34);
- Cent2: Center of the $Cp^{*}$ ring (C20~C24).

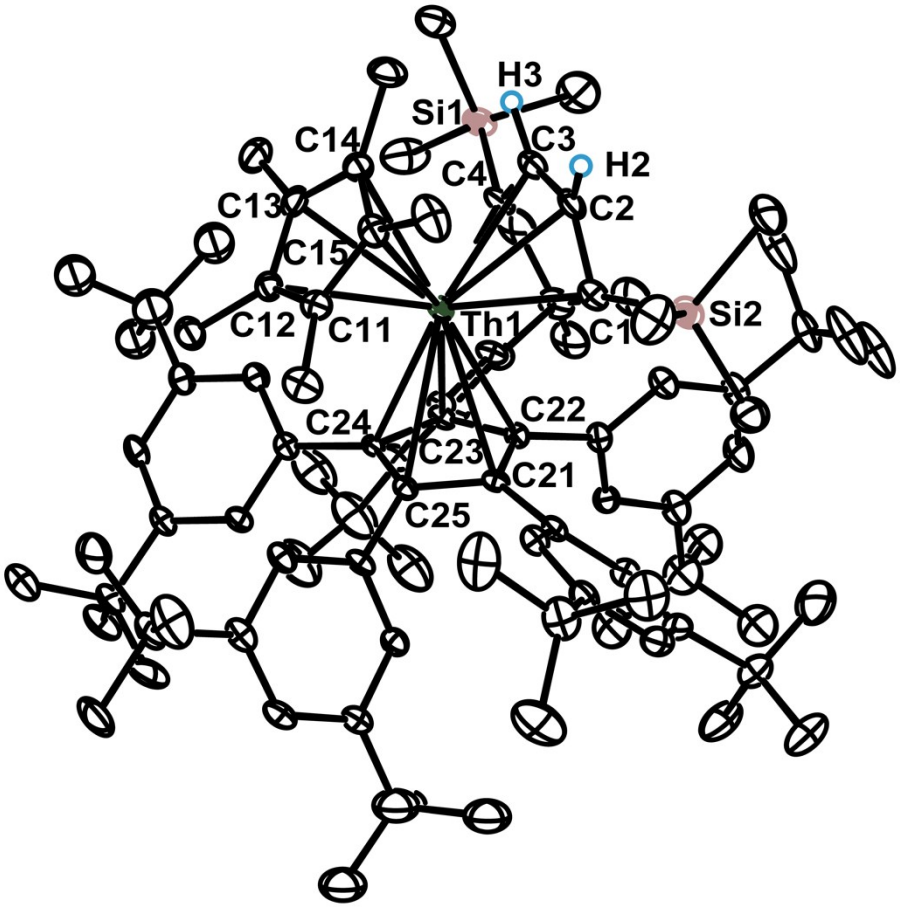



**Figure S19.** ORTEP plot (30% probability) of [($Cp^{Ar*}$)($Cp^{*}$)Th($Me_3SiC{\equiv}CH{\equiv}CH{\equiv}C{\equiv}SiMe_3$] **(5)**. All the hydrogen atoms, except H2 and H3, are omitted for clarity. Selected interatomic distances [Å] and angles [deg]: C1—C2 1.451(8), C2—C3 1.375(8), C3—C4 1.471(7), Th1—C1 2.544(5), Th1—C2 2.666(5), Th1—C3 2.674(5), Th1—C4 2.529(5), Th1—C11 2.829(5), Th1—C12 2.818(5), Th1—C13 2.821(5), Th1—C14 2.843(5), Th1—C15 2.832(5), Th1—C21 2.892(5), Th1—C22 2.938(5), Th1—C23 3.014(4), Th1—C24 2.953(4), Th1—C25 2.917(4), Th1—Cent1 2.682, Th1—Cent2 2.557; C4—C3—C2 130.7(5), C3—C2—C1 132.5(5), Cent1—Th1—Cent2 132.47.

- Cent1: Centre of the $Cp^{Ar*}$ ring (C21~C25);
- Cent2: Center of the $Cp^{*}$ ring (C11~C15).

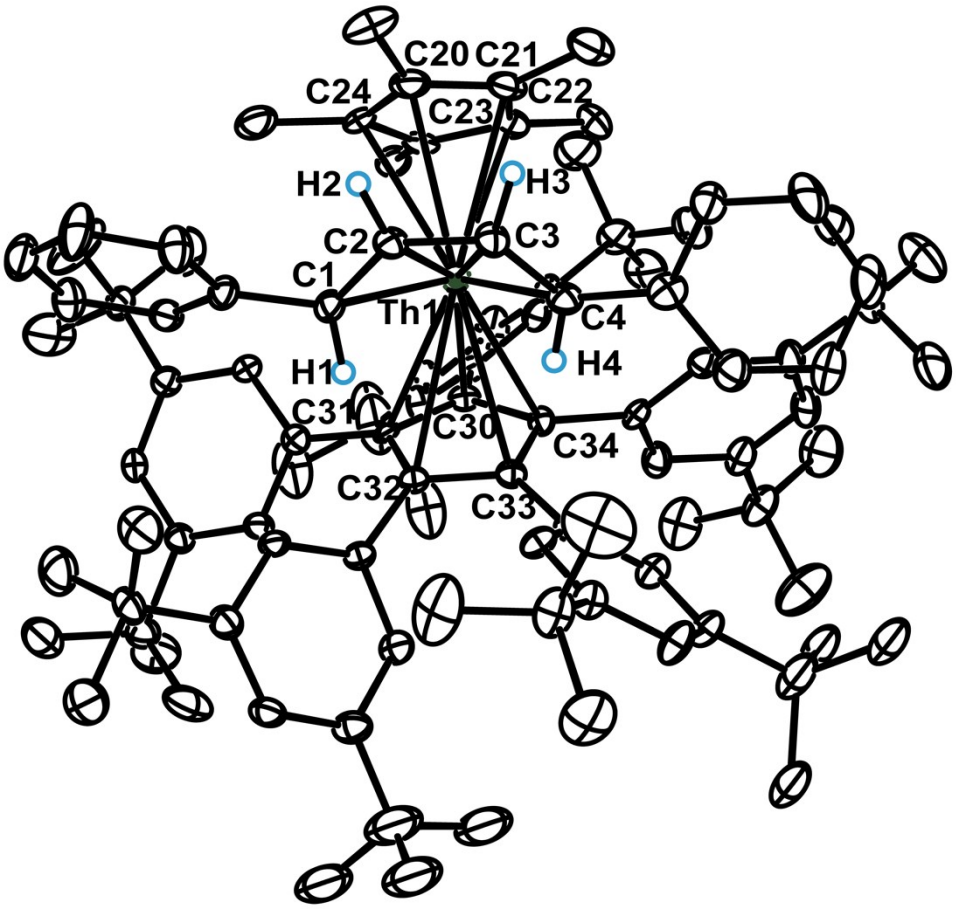



**Figure S20.** ORTEP plot (30% probability) of [($Cp^{Ar*}$)($Cp^{*}$)Th(PhCH-CH=CH-CHPh)] (**6**). All the hydrogen atoms, except H1, H2, H3 and H4, are omitted for clarity. Selected interatomic distances [Å] and angles [deg]: C1—C2 1.429(7), C2—C3 1.389(7), C3—C4 1.398(7), Th1—C1 2.501(5), Th1—C2 2.674(5), Th1—C3 2.699(5), Th1—C4 2.562(5), Th1—C20 2.853(6), Th1—C21 2.840(5), Th1—C22 2.769(5) 2.769(5), Th1—C23 2.755(5), Th1—C24 2.793(5), Th1—C30 2.944(5), Th1—C31 3.004(5), Th1—C32 3.017(5), Th1—C33 2.969(5), Th1—C34 2.890(5), Th1—Cent1 2.706, Th1—Cent2 2.526; C4—C3—C2 131.6(5), C3—C2—C1 131.8(6), Cent1—Th1—Cent2 135.21.

- Cent1: Centre of the $Cp^{Ar*}$ ring (C30~C34);
- Cent2: Center of the $Cp^{*}$ ring (C20~C24).

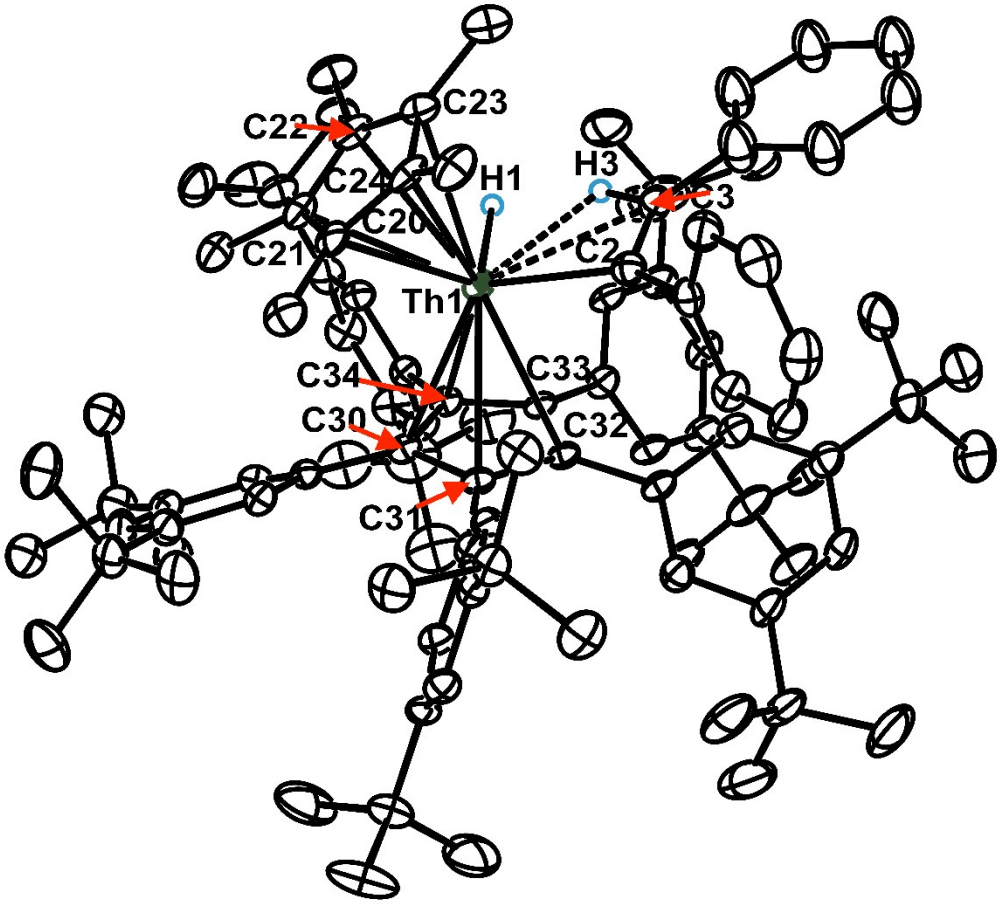



**Figure S21.** ORTEP plot (30% probability) of [($Cp^{Ar*}$)($Cp^{*}$)ThH(PhC=CHPh)] (**7**). All the hydrogen atoms, except H1 and H3, are omitted for clarity. Selected interatomic distances [Å] and angles [deg]: C2—C3 1.336(7), Th1—H1 2.20(5), Th1—H3 2.21(4), Th1—C2 2.475(5), Th1—C3 2.778(5), Th1—C20 2.774(5), Th1—C21 2.779(5), Th1—C22 2.810(5), Th1—C23 2.809(5), Th1—C24 2.801(5), Th1—C30 2.846(5), Th1—C31 2.821(4), Th1—C32 2.905(4), Th1—C33 2.909(4), Th1—C34 2.872(4), Th1—Cent1 2.601, Th1—Cent2 2.522; Cent1—Th1—Cent2 142.15.

- Cent1: Centre of the $Cp^{Ar*}$ ring (C30~C34);
- Cent2: Center of the $Cp^{*}$ ring (C20~C24).

## 6. Computational details.

All DFT calculations were carried out with the Gaussian 09 suite of programs.[14] Geometries were fully optimized in gas phase without symmetry constraints, employing the B3PW91 functional.[15] The nature of the extrema was verified by analytical frequency calculations. The calculation of electronic energies and enthalpies of the extrema of the potential energy surface (minima and transition states) were performed at the same level of theory as the geometry optimizations. IRC calculations were performed to confirm the connections of the optimized transition states. Thorium atoms were treated with a small core effective core potential (60MWB), associated with its adapted basis set.[16] For the other elements (H, C, and O), Pople's double-ζ basis set 6-31G(d,p) was used.[17] The electronic charges (at the DFT level) were computed using the natural population analysis (NPA) technique.[18]

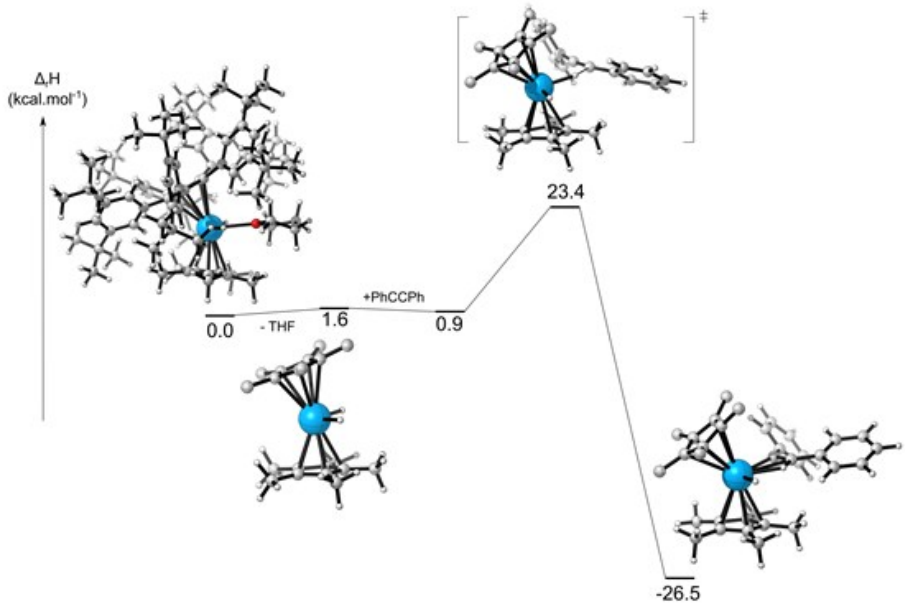



**Figure S22.** Computed Enthalpy profile for the formation of complex **7** at room temperature

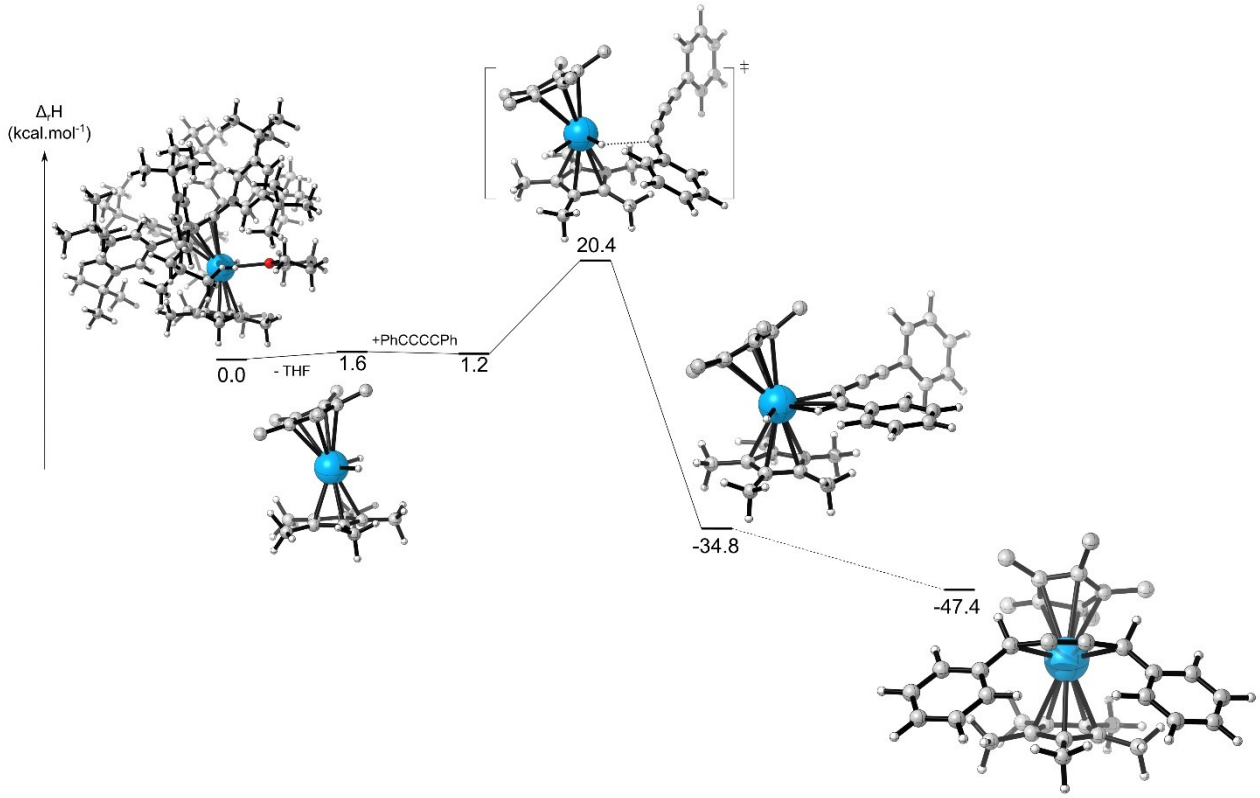



**Figure S23.** Computed Enthalpy profile for the formation of complex **4** at room temperature

**Cartesian coordinates of all optimized structures**

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Initial complex with THF

| | | | |
|---|---|---|---|
| O | 14.46321 | 3.85373 | 3.19927 |
| C | 14.26745 | 4.71178 | 2.04509 |
| H | 14.35541 | 4.09513 | 1.14607 |
| H | 13.25216 | 5.10461 | 2.08306 |
| C | 15.35871 | 5.77364 | 2.11657 |
| H | 15.01978 | 6.63821 | 2.69648 |
| H | 15.64970 | 6.12767 | 1.12370 |
| C | 16.47927 | 5.04534 | 2.85893 |
| H | 17.03500 | 4.39202 | 2.17802 |
| H | 17.19140 | 5.72160 | 3.33989 |
| C | 15.69713 | 4.22464 | 3.87039 |
| H | 16.17693 | 3.29993 | 4.18961 |
| H | 15.43570 | 4.81051 | 4.75794 |
| C | 12.63119 | -0.10450 | 1.83954 |
| C | 13.49461 | 0.85478 | 1.23398 |
| C | 14.75422 | 0.78212 | 1.89493 |
| C | 14.67331 | -0.21389 | 2.90411 |
| C | 13.36280 | -0.76941 | 2.86944 |
| C | 11.25121 | -0.44878 | 1.35212 |
| H | 11.06721 | 0.00144 | 0.37369 |
| H | 11.13956 | -1.53232 | 1.23496 |
| H | 10.44125 | -0.10770 | 2.00856 |
| C | 13.19317 | 1.61952 | -0.02399 |
| H | 12.19202 | 2.05563 | -0.01605 |
| H | 13.89960 | 2.43917 | -0.17834 |
| H | 13.27152 | 0.96504 | -0.90319 |
| C | 16.01820 | 1.47948 | 1.49062 |
| H | 16.65482 | 1.69617 | 2.35350 |
| H | 16.60606 | 0.85196 | 0.80724 |
| H | 15.82583 | 2.42100 | 0.97032 |
| C | 15.82037 | -0.74543 | 3.70970 |
| H | 15.48027 | -1.21485 | 4.63642 |
| H | 16.37171 | -1.51178 | 3.14647 |
| H | 16.52733 | 0.04117 | 3.98386 |
| C | 12.93105 | -1.98646 | 3.63637 |
| H | 13.06221 | -1.89239 | 4.71999 |
| H | 11.87694 | -2.20977 | 3.46856 |
| H | 13.51023 | -2.86320 | 3.31850 |
| C | 11.03756 | 1.04110 | 5.94159 |
| C | 12.09744 | 1.74484 | 6.61300 |

| | | | |
|---|---|---|---|
| C | 12.02257 | 3.12866 | 6.25012 |
| C | 10.92976 | 3.28589 | 5.33654 |
| C | 10.33043 | 2.00086 | 5.13935 |
| C | 10.57046 | -0.34399 | 6.24057 |
| C | 10.55995 | -0.79168 | 7.56816 |
| H | 10.94549 | -0.13519 | 8.33889 |
| C | 10.04386 | -2.04319 | 7.92917 |
| C | 10.03648 | -2.46867 | 9.40498 |
| C | 9.28464 | -1.41418 | 10.24054 |
| H | 9.27524 | -1.70314 | 11.29804 |
| H | 9.75288 | -0.42835 | 10.16899 |
| H | 8.24618 | -1.31679 | 9.90653 |
| C | 9.34585 | -3.82242 | 9.62247 |
| H | 9.35358 | -4.07035 | 10.68915 |
| H | 8.30095 | -3.80517 | 9.29427 |
| H | 9.85903 | -4.63383 | 9.09525 |
| C | 11.48735 | -2.58228 | 9.90899 |
| H | 11.50334 | -2.85933 | 10.96987 |
| H | 12.03008 | -3.35267 | 9.35071 |
| H | 12.03256 | -1.64114 | 9.79665 |
| C | 9.53558 | -2.85425 | 6.91670 |
| H | 9.13940 | -3.83030 | 7.17207 |
| C | 9.50217 | -2.44747 | 5.57427 |
| C | 8.90837 | -3.40965 | 4.53119 |
| C | 9.84710 | -4.62261 | 4.37041 |
| H | 10.83710 | -4.31561 | 4.01914 |
| H | 9.98078 | -5.15196 | 5.31923 |
| H | 9.43449 | -5.33285 | 3.64400 |
| C | 8.72394 | -2.74491 | 3.16174 |
| H | 9.67928 | -2.45646 | 2.71567 |
| H | 8.24391 | -3.44625 | 2.47084 |
| H | 8.09663 | -1.84982 | 3.22486 |
| C | 7.52867 | -3.91794 | 4.99555 |
| H | 6.83725 | -3.08774 | 5.16636 |
| H | 7.09317 | -4.57066 | 4.23039 |
| H | 7.58840 | -4.49799 | 5.92088 |
| C | 10.02448 | -1.19091 | 5.25532 |
| H | 9.99242 | -0.83764 | 4.23069 |
| C | 12.92815 | 1.23337 | 7.74127 |
| C | 13.93027 | 0.27526 | 7.59947 |
| H | 14.16481 | -0.08699 | 6.60273 |
| C | 14.65411 | -0.19943 | 8.70700 |
| C | 15.76851 | -1.23752 | 8.50556 |
| C | 15.21047 | -2.46660 | 7.76316 |
| H | 14.80989 | -2.20623 | 6.77951 |
| H | 16.00082 | -3.21087 | 7.61216 |

| | | | |
|---|---|---|---|
| H | 14.40401 | -2.93628 | 8.33471 |
| C | 16.90108 | -0.60597 | 7.67276 |
| H | 16.53587 | -0.22945 | 6.71335 |
| H | 17.35535 | 0.23446 | 8.20777 |
| H | 17.68661 | -1.34443 | 7.47265 |
| C | 16.36633 | -1.72560 | 9.83312 |
| H | 16.83843 | -0.91271 | 10.39505 |
| H | 15.61032 | -2.19331 | 10.47311 |
| H | 17.13995 | -2.47442 | 9.63271 |
| C | 14.33747 | 0.31845 | 9.96393 |
| H | 14.88344 | -0.03672 | 10.83120 |
| C | 13.33490 | 1.28507 | 10.15275 |
| C | 13.04036 | 1.80950 | 11.56639 |
| C | 14.28922 | 2.52544 | 12.11644 |
| H | 14.10684 | 2.88271 | 13.13681 |
| H | 15.15877 | 1.86155 | 12.14599 |
| H | 14.54576 | 3.38967 | 11.49593 |
| C | 12.68054 | 0.63431 | 12.49592 |
| H | 12.47035 | 1.00205 | 13.50691 |
| H | 11.79201 | 0.10672 | 12.13501 |
| H | 13.49378 | -0.09376 | 12.57076 |
| C | 11.87328 | 2.80636 | 11.58453 |
| H | 11.70125 | 3.15324 | 12.60913 |
| H | 12.07988 | 3.68575 | 10.96648 |
| H | 10.94277 | 2.34996 | 11.23016 |
| C | 12.64678 | 1.73181 | 9.02668 |
| H | 11.86737 | 2.47967 | 9.11895 |
| C | 12.81248 | 4.20896 | 6.90309 |
| C | 14.19778 | 4.07670 | 7.11594 |
| H | 14.68767 | 3.19436 | 6.71731 |
| C | 14.92162 | 5.04335 | 7.81625 |
| C | 16.43533 | 4.93416 | 8.06358 |
| C | 17.01061 | 3.60015 | 7.57171 |
| H | 18.08367 | 3.55782 | 7.78866 |
| H | 16.53171 | 2.75080 | 8.06817 |
| H | 16.88605 | 3.46819 | 6.49311 |
| C | 17.15644 | 6.08382 | 7.33241 |
| H | 16.80720 | 7.06281 | 7.67554 |
| H | 18.23747 | 6.03226 | 7.50792 |
| H | 16.98706 | 6.03179 | 6.25162 |
| C | 16.73321 | 5.04081 | 9.57205 |
| H | 16.38614 | 5.98688 | 9.99804 |
| H | 16.25164 | 4.22625 | 10.12124 |
| H | 17.81316 | 4.97585 | 9.74925 |
| C | 14.22960 | 6.16136 | 8.30836 |
| H | 14.78605 | 6.91636 | 8.85293 |

| | | | |
|---|---|---|---|
| C | 12.85561 | 6.32547 | 8.13233 |
| C | 12.08719 | 7.52219 | 8.71446 |
| C | 11.41468 | 8.30987 | 7.57504 |
| H | 10.73495 | 7.68517 | 6.98900 |
| H | 10.83826 | 9.14984 | 7.98113 |
| H | 12.16727 | 8.71642 | 6.89136 |
| C | 12.99945 | 8.48607 | 9.48617 |
| H | 13.48889 | 7.99555 | 10.33440 |
| H | 13.77554 | 8.91620 | 8.84386 |
| H | 12.40503 | 9.31584 | 9.88341 |
| C | 11.00634 | 7.01008 | 9.68684 |
| H | 11.45724 | 6.45628 | 10.51718 |
| H | 10.44250 | 7.85108 | 10.10729 |
| H | 10.29372 | 6.34578 | 9.18955 |
| C | 12.16313 | 5.33606 | 7.41886 |
| H | 11.09169 | 5.42776 | 7.27746 |
| C | 10.27489 | 4.57572 | 4.96777 |
| C | 10.85388 | 5.54528 | 4.14474 |
| H | 11.81218 | 5.31723 | 3.69023 |
| C | 10.21418 | 6.76598 | 3.88830 |
| C | 10.86111 | 7.79308 | 2.94562 |
| C | 12.28409 | 8.12435 | 3.43130 |
| H | 12.25913 | 8.58828 | 4.42200 |
| H | 12.90855 | 7.23020 | 3.50542 |
| H | 12.77140 | 8.82198 | 2.73990 |
| C | 10.07409 | 9.10976 | 2.87463 |
| H | 9.98933 | 9.58735 | 3.85650 |
| H | 10.59024 | 9.80993 | 2.20892 |
| H | 9.06530 | 8.96314 | 2.47496 |
| C | 10.92299 | 7.20080 | 1.52409 |
| H | 11.46387 | 6.25031 | 1.50372 |
| H | 9.91596 | 7.01133 | 1.13880 |
| H | 11.42442 | 7.89461 | 0.83863 |
| C | 8.97277 | 6.99868 | 4.49076 |
| H | 8.47043 | 7.93941 | 4.30659 |
| C | 8.35691 | 6.05566 | 5.32202 |
| C | 6.98853 | 6.30274 | 5.97402 |
| C | 6.45008 | 7.71311 | 5.69569 |
| H | 5.48135 | 7.84098 | 6.19049 |
| H | 7.12173 | 8.48951 | 6.07782 |
| H | 6.29599 | 7.88858 | 4.62573 |
| C | 5.97799 | 5.28148 | 5.41896 |
| H | 5.00012 | 5.40923 | 5.89844 |
| H | 5.84654 | 5.40926 | 4.33963 |
| H | 6.31043 | 4.25375 | 5.58826 |
| C | 7.10034 | 6.13018 | 7.50136 |

| | | | |
|---|---|---|---|
| H | 6.12749 | 6.30162 | 7.97659 |
| H | 7.42930 | 5.12359 | 7.77545 |
| H | 7.81471 | 6.84402 | 7.92476 |
| C | 9.02487 | 4.84756 | 5.54202 |
| H | 8.57942 | 4.08728 | 6.17707 |
| C | 9.05076 | 1.80921 | 4.40554 |
| C | 7.94848 | 1.22216 | 5.05445 |
| H | 8.08459 | 0.85737 | 6.06589 |
| C | 6.70639 | 1.12156 | 4.42835 |
| C | 5.47640 | 0.50538 | 5.11398 |
| C | 4.38364 | 1.57957 | 5.28134 |
| H | 3.48882 | 1.14357 | 5.74088 |
| H | 4.72930 | 2.39618 | 5.92251 |
| H | 4.08893 | 2.01151 | 4.31995 |
| C | 5.80781 | -0.06141 | 6.50120 |
| H | 4.91168 | -0.51476 | 6.93854 |
| H | 6.58457 | -0.83144 | 6.45447 |
| H | 6.14808 | 0.72061 | 7.18830 |
| C | 4.91632 | -0.63704 | 4.24418 |
| H | 4.04856 | -1.09647 | 4.73168 |
| H | 4.59258 | -0.28128 | 3.26142 |
| H | 5.66733 | -1.41619 | 4.08328 |
| C | 6.58435 | 1.62728 | 3.12230 |
| H | 5.61990 | 1.55972 | 2.63032 |
| C | 7.64965 | 2.22040 | 2.44545 |
| C | 7.50489 | 2.80786 | 1.03416 |
| C | 7.75148 | 4.32784 | 1.09798 |
| H | 7.01432 | 4.81589 | 1.74358 |
| H | 8.74326 | 4.55801 | 1.49661 |
| H | 7.67534 | 4.76959 | 0.09707 |
| C | 8.54255 | 2.16695 | 0.09339 |
| H | 8.39205 | 1.08442 | 0.02280 |
| H | 8.45356 | 2.58885 | -0.91460 |
| H | 9.56438 | 2.34520 | 0.44029 |
| C | 6.11098 | 2.57028 | 0.43713 |
| H | 5.87696 | 1.50294 | 0.35866 |
| H | 5.32487 | 3.05243 | 1.02802 |
| H | 6.06733 | 2.99330 | -0.57212 |
| C | 8.88515 | 2.30116 | 3.10801 |
| H | 9.73919 | 2.77276 | 2.62556 |
| Th | 12.92155 | 1.79107 | 3.84229 |
| H | 14.71064 | 1.85879 | 4.91965 |
| H | 12.04873 | 3.12868 | 2.47852 |

13

THF

| | | | |
|---|---|---|---|
| C | -0.18412 | 1.73579 | 0.46953 |

| | | | |
|---|---|---|---|
| C | 0.73348 | 2.34954 | 1.52888 |
| C | 1.91627 | 2.81626 | 0.67674 |
| C | 1.99716 | 1.69510 | -0.35682 |
| O | 0.66037 | 1.25689 | -0.57442 |
| H | -0.87601 | 2.48833 | 0.06131 |
| H | -0.78474 | 0.90323 | 0.85569 |
| H | 1.06028 | 1.58508 | 2.24319 |
| H | 0.25267 | 3.15430 | 2.09207 |
| H | 2.84280 | 2.94241 | 1.24404 |
| H | 1.68251 | 3.76965 | 0.18904 |
| H | 2.60933 | 0.85987 | 0.01985 |
| H | 2.42112 | 2.01732 | -1.31483 |

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Intital complex without THF

| | | | |
|---|---|---|---|
| C | 12.63970 | 0.04811 | 1.74384 |
| C | 13.32895 | 1.23579 | 1.36455 |
| C | 14.57841 | 1.24961 | 2.04491 |
| C | 14.68131 | 0.05996 | 2.82023 |
| C | 13.47693 | -0.68022 | 2.64446 |
| C | 11.32352 | -0.42436 | 1.18903 |
| H | 11.09984 | 0.07565 | 0.24303 |
| H | 11.35038 | -1.50150 | 0.99084 |
| H | 10.46270 | -0.24655 | 1.84835 |
| C | 12.88111 | 2.21759 | 0.32170 |
| H | 11.80106 | 2.38612 | 0.34485 |
| H | 13.35864 | 3.19001 | 0.45832 |
| H | 13.13436 | 1.85779 | -0.68510 |
| C | 15.63718 | 2.30446 | 1.91847 |
| H | 16.23481 | 2.38217 | 2.83151 |
| H | 16.32710 | 2.08222 | 1.09369 |
| H | 15.20180 | 3.28925 | 1.72551 |
| C | 15.90644 | -0.40369 | 3.55146 |
| H | 15.66297 | -1.04890 | 4.39983 |
| H | 16.56339 | -0.97772 | 2.88372 |
| H | 16.48146 | 0.43753 | 3.94465 |
| C | 13.18839 | -2.05079 | 3.19274 |
| H | 14.05319 | -2.45021 | 3.72845 |
| H | 12.33794 | -2.08079 | 3.88582 |
| H | 12.95850 | -2.75346 | 2.38190 |
| C | 10.84746 | 1.00773 | 6.13234 |
| C | 11.91008 | 1.71081 | 6.79504 |
| C | 11.86673 | 3.07645 | 6.37906 |
| C | 10.78597 | 3.23069 | 5.45720 |
| C | 10.15844 | 1.95296 | 5.29651 |
| C | 10.43428 | -0.39525 | 6.40275 |
| C | 10.35553 | -0.83683 | 7.72835 |

| | | | |
|---|---|---|---|
| H | 10.63190 | -0.14687 | 8.51780 |
| C | 9.91124 | -2.12373 | 8.05626 |
| C | 9.81211 | -2.54088 | 9.53084 |
| C | 8.88516 | -1.56121 | 10.27768 |
| H | 8.80153 | -1.84832 | 11.33219 |
| H | 9.26142 | -0.53473 | 10.24235 |
| H | 7.87949 | -1.56506 | 9.84409 |
| C | 9.24316 | -3.95592 | 9.70425 |
| H | 9.18659 | -4.19924 | 10.77038 |
| H | 8.23211 | -4.04454 | 9.29195 |
| H | 9.87643 | -4.71314 | 9.22955 |
| C | 11.21406 | -2.50497 | 10.16779 |
| H | 11.15505 | -2.76081 | 11.23226 |
| H | 11.87751 | -3.22926 | 9.68360 |
| H | 11.67944 | -1.51919 | 10.08227 |
| C | 9.55444 | -2.97406 | 7.00974 |
| H | 9.21412 | -3.97741 | 7.23971 |
| C | 9.60237 | -2.57692 | 5.66442 |
| C | 9.16704 | -3.57911 | 4.58302 |
| C | 10.15961 | -4.75866 | 4.55655 |
| H | 11.17277 | -4.41765 | 4.32121 |
| H | 10.19833 | -5.27377 | 5.52149 |
| H | 9.86250 | -5.49117 | 3.79700 |
| C | 9.12086 | -2.94747 | 3.18677 |
| H | 10.10866 | -2.61171 | 2.85897 |
| H | 8.76999 | -3.68582 | 2.45801 |
| H | 8.43801 | -2.09199 | 3.15090 |
| C | 7.75898 | -4.11968 | 4.90115 |
| H | 7.02657 | -3.30781 | 4.94518 |
| H | 7.44105 | -4.82202 | 4.12221 |
| H | 7.72421 | -4.65177 | 5.85603 |
| C | 10.04628 | -1.28223 | 5.37926 |
| H | 10.05814 | -0.93028 | 4.35157 |
| C | 12.77213 | 1.19101 | 7.89212 |
| C | 13.68718 | 0.15361 | 7.71648 |
| H | 13.81854 | -0.26365 | 6.72233 |
| C | 14.46327 | -0.33186 | 8.77988 |
| C | 15.50924 | -1.42825 | 8.52707 |
| C | 14.88103 | -2.60385 | 7.75587 |
| H | 14.49289 | -2.29905 | 6.77996 |
| H | 15.63062 | -3.38428 | 7.58226 |
| H | 14.05295 | -3.04600 | 8.31851 |
| C | 16.65684 | -0.82507 | 7.69268 |
| H | 16.29058 | -0.41067 | 6.74891 |
| H | 17.15104 | -0.01495 | 8.23926 |
| H | 17.40966 | -1.58878 | 7.46320 |

| | | | |
|---|---|---|---|
| C | 16.10105 | -1.98604 | 9.82989 |
| H | 16.64788 | -1.22287 | 10.39303 |
| H | 15.32654 | -2.40555 | 10.48106 |
| H | 16.81103 | -2.78676 | 9.59713 |
| C | 14.28433 | 0.25364 | 10.03432 |
| H | 14.87298 | -0.10482 | 10.87164 |
| C | 13.37384 | 1.29966 | 10.25694 |
| C | 13.24404 | 1.90267 | 11.66337 |
| C | 14.59702 | 2.51233 | 12.08105 |
| H | 14.52743 | 2.94249 | 13.08705 |
| H | 15.39442 | 1.76276 | 12.09370 |
| H | 14.89494 | 3.30758 | 11.39035 |
| C | 12.85008 | 0.80263 | 12.66809 |
| H | 12.76395 | 1.22290 | 13.67681 |
| H | 11.88558 | 0.35717 | 12.40323 |
| H | 13.59022 | -0.00249 | 12.70630 |
| C | 12.18225 | 3.00891 | 11.72608 |
| H | 12.12833 | 3.40997 | 12.74388 |
| H | 12.41996 | 3.83950 | 11.05398 |
| H | 11.18678 | 2.63265 | 11.46674 |
| C | 12.62758 | 1.75534 | 9.17096 |
| H | 11.91529 | 2.56318 | 9.29264 |
| C | 12.70098 | 4.17107 | 6.94163 |
| C | 14.10300 | 4.10043 | 6.93367 |
| H | 14.56543 | 3.23814 | 6.46431 |
| C | 14.87956 | 5.10849 | 7.50514 |
| C | 16.41475 | 5.07925 | 7.48333 |
| C | 16.96195 | 3.81761 | 6.80245 |
| H | 18.05724 | 3.83976 | 6.81196 |
| H | 16.64121 | 2.90636 | 7.31691 |
| H | 16.63914 | 3.74564 | 5.75891 |
| C | 16.93448 | 6.30749 | 6.71018 |
| H | 16.61321 | 7.24606 | 7.17236 |
| H | 18.03053 | 6.30678 | 6.68215 |
| H | 16.56788 | 6.30131 | 5.67830 |
| C | 16.95656 | 5.11717 | 8.92568 |
| H | 16.63404 | 6.01506 | 9.46192 |
| H | 16.61286 | 4.24607 | 9.49294 |
| H | 18.05284 | 5.10873 | 8.92130 |
| C | 14.21895 | 6.18885 | 8.11114 |
| H | 14.81760 | 6.97117 | 8.56569 |
| C | 12.82704 | 6.29174 | 8.14812 |
| C | 12.10202 | 7.47438 | 8.80890 |
| C | 11.34444 | 8.27089 | 7.72947 |
| H | 10.63175 | 7.64420 | 7.18594 |
| H | 10.79174 | 9.10180 | 8.18440 |

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| H | 12.04251 | 8.69046 | 6.99777 |
| C | 13.06868 | 8.43136 | 9.52120 |
| H | 13.63686 | 7.92542 | 10.30941 |
| H | 13.77990 | 8.88922 | 8.82547 |
| H | 12.50285 | 9.24367 | 9.98983 |
| C | 11.09669 | 6.95396 | 9.85427 |
| H | 11.60564 | 6.38620 | 10.64017 |
| H | 10.57333 | 7.79267 | 10.32773 |
| H | 10.33997 | 6.30312 | 9.40668 |
| C | 12.08129 | 5.27000 | 7.54338 |
| H | 10.99678 | 5.31802 | 7.54237 |
| C | 10.22275 | 4.53577 | 5.00633 |
| C | 10.93428 | 5.44126 | 4.21513 |
| H | 11.90897 | 5.13894 | 3.84760 |
| C | 10.40187 | 6.68842 | 3.87062 |
| C | 11.21424 | 7.62585 | 2.96413 |
| C | 12.59546 | 7.89337 | 3.59262 |
| H | 12.49458 | 8.37937 | 4.56785 |
| H | 13.16344 | 6.97055 | 3.73981 |
| H | 13.18640 | 8.55020 | 2.94354 |
| C | 10.52186 | 8.97754 | 2.74322 |
| H | 10.36558 | 9.51389 | 3.68551 |
| H | 11.14605 | 9.61016 | 2.10314 |
| H | 9.55192 | 8.86592 | 2.24674 |
| C | 11.40769 | 6.95170 | 1.59091 |
| H | 11.92549 | 5.99218 | 1.68395 |
| H | 10.44251 | 6.76737 | 1.10699 |
| H | 12.00144 | 7.59425 | 0.92976 |
| C | 9.13088 | 7.02064 | 4.35533 |
| H | 8.70955 | 7.98536 | 4.10301 |
| C | 8.38645 | 6.14455 | 5.15627 |
| C | 6.99583 | 6.50424 | 5.70369 |
| C | 6.55362 | 7.91865 | 5.30380 |
| H | 5.56347 | 8.12599 | 5.72362 |
| H | 7.23971 | 8.68354 | 5.68297 |
| H | 6.47978 | 8.03248 | 4.21702 |
| C | 5.95662 | 5.50469 | 5.16072 |
| H | 4.96304 | 5.72666 | 5.56788 |
| H | 5.89488 | 5.56105 | 4.06912 |
| H | 6.20754 | 4.47331 | 5.42412 |
| C | 7.01388 | 6.43009 | 7.24328 |
| H | 6.02614 | 6.67904 | 7.64875 |
| H | 7.27637 | 5.42961 | 7.60009 |
| H | 7.73894 | 7.13646 | 7.66089 |
| C | 8.94947 | 4.90162 | 5.46405 |
| H | 8.40248 | 4.19477 | 6.08187 |

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| C | 8.91070 | 1.73981 | 4.52090 |
| C | 7.81455 | 1.08573 | 5.11202 |
| H | 7.93243 | 0.69390 | 6.11530 |
| C | 6.59672 | 0.96502 | 4.44527 |
| C | 5.36850 | 0.29231 | 5.07652 |
| C | 4.24853 | 1.33773 | 5.24858 |
| H | 3.35717 | 0.87368 | 5.68648 |
| H | 4.56871 | 2.14909 | 5.91012 |
| H | 3.95797 | 1.78219 | 4.29169 |
| C | 5.67857 | -0.31119 | 6.45299 |
| H | 4.78413 | -0.80343 | 6.84954 |
| H | 6.47670 | -1.05893 | 6.40130 |
| H | 5.97795 | 0.45553 | 7.17531 |
| C | 4.86376 | -0.83666 | 4.15687 |
| H | 3.99102 | -1.32767 | 4.60240 |
| H | 4.56528 | -0.46193 | 3.17320 |
| H | 5.63754 | -1.59521 | 4.00202 |
| C | 6.49227 | 1.51444 | 3.15574 |
| H | 5.54354 | 1.43499 | 2.63649 |
| C | 7.55239 | 2.17009 | 2.53051 |
| C | 7.42526 | 2.79336 | 1.13253 |
| C | 7.72491 | 4.30257 | 1.21563 |
| H | 7.01095 | 4.80591 | 1.87461 |
| H | 8.72707 | 4.50314 | 1.60437 |
| H | 7.65241 | 4.75906 | 0.22146 |
| C | 8.43444 | 2.12635 | 0.17955 |
| H | 8.24221 | 1.05165 | 0.09293 |
| H | 8.36468 | 2.56702 | -0.82165 |
| H | 9.46215 | 2.25794 | 0.52961 |
| C | 6.02193 | 2.61750 | 0.53555 |
| H | 5.75756 | 1.56163 | 0.41192 |
| H | 5.25329 | 3.09558 | 1.15200 |
| H | 5.98536 | 3.08310 | -0.45487 |
| C | 8.76364 | 2.26895 | 3.23400 |
| H | 9.59996 | 2.80840 | 2.79385 |
| Th | 12.65237 | 1.54003 | 4.04667 |
| H | 14.41960 | 1.63247 | 5.09529 |
| H | 12.59013 | 3.34353 | 3.05230 |

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PhCCPh

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|---|---|---|---|
| C | 8.61306 | 10.12579 | 11.64498 |
| C | 9.09367 | 9.08495 | 11.23576 |
| C | 9.65595 | 7.86884 | 10.75783 |
| C | 11.03082 | 7.60814 | 10.90946 |
| C | 11.57596 | 6.41823 | 10.44102 |
| C | 10.76553 | 5.47009 | 9.81564 |

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| C | 9.40145 | 5.71897 | 9.66039 |
| C | 8.84705 | 6.90594 | 10.12553 |
| C | 8.05079 | 11.34192 | 12.12286 |
| C | 8.85961 | 12.30474 | 12.75533 |
| C | 8.30518 | 13.49172 | 13.22046 |
| C | 6.94114 | 13.74065 | 13.06503 |
| C | 6.13078 | 12.79259 | 12.43943 |
| C | 6.67593 | 11.60269 | 11.97101 |
| H | 6.04880 | 10.86254 | 11.48378 |
| H | 5.06799 | 12.98161 | 12.31601 |
| H | 6.51152 | 14.66938 | 13.42978 |
| H | 8.94053 | 14.22673 | 13.70685 |
| H | 9.92047 | 12.10747 | 12.87432 |
| H | 11.65803 | 8.34834 | 11.39651 |
| H | 12.63878 | 6.22930 | 10.56426 |
| H | 11.19512 | 4.54135 | 9.45089 |
| H | 8.76607 | 4.98389 | 9.17413 |

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PhCCPh adduct

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| C | 13.91133 | 11.15898 | 6.82049 |
| C | 13.92157 | 10.86139 | 8.18473 |
| C | 12.82493 | 11.12614 | 9.02098 |
| C | 10.45420 | 12.65246 | 6.43780 |
| C | 10.00896 | 13.99473 | 6.64181 |
| C | 9.05089 | 14.31114 | 5.62667 |
| C | 8.88916 | 13.15334 | 4.79582 |
| C | 9.75466 | 12.12650 | 5.30289 |
| Th | 7.71616 | 12.39925 | 7.26850 |
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| C | 5.16761 | 11.34752 | 7.18891 |
| C | 5.14416 | 12.18174 | 8.34456 |
| C | 5.99902 | 11.59686 | 9.32170 |
| C | 6.53868 | 10.39758 | 8.78050 |
| C | 4.31991 | 11.54386 | 5.96462 |
| C | 4.22821 | 13.34967 | 8.56486 |
| C | 6.21019 | 12.11011 | 10.71493 |
| C | 7.40821 | 9.41400 | 9.50649 |
| C | 6.26600 | 9.04905 | 6.56922 |
| C | 8.54866 | 15.68332 | 5.33511 |
| C | 7.19531 | 16.01339 | 5.27923 |
| C | 6.76719 | 17.31335 | 4.97173 |
| C | 7.74315 | 18.27546 | 4.70535 |
| C | 9.11711 | 17.98513 | 4.74265 |

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| C | 9.49869 | 16.68243 | 5.06088 |
| C | 10.49180 | 14.94400 | 7.67445 |
| C | 9.57793 | 15.68629 | 8.43513 |
| C | 10.01098 | 16.60635 | 9.39420 |
| C | 11.39011 | 16.77820 | 9.55731 |
| C | 12.33572 | 16.06449 | 8.81111 |
| C | 11.86509 | 15.14115 | 7.87315 |
| C | 10.05444 | 10.81719 | 4.66838 |
| C | 10.36670 | 10.75888 | 3.30684 |
| C | 10.75832 | 9.56182 | 2.69165 |
| C | 10.80117 | 8.40945 | 3.47865 |
| C | 10.49068 | 8.41773 | 4.84763 |
| C | 10.12587 | 9.63482 | 5.42659 |
| C | 8.12064 | 13.09741 | 3.52374 |
| C | 8.28755 | 14.12204 | 2.58544 |
| C | 7.64357 | 14.09746 | 1.34247 |
| C | 6.80489 | 13.01666 | 1.06483 |
| C | 6.61536 | 11.95715 | 1.96535 |
| C | 7.28563 | 12.01514 | 3.19145 |
| C | 9.03666 | 17.41955 | 10.25878 |
| C | 9.25921 | 18.92452 | 10.01073 |
| C | 13.83286 | 16.32306 | 9.03877 |
| C | 14.18691 | 16.03963 | 10.51175 |
| C | 5.26618 | 17.63960 | 4.98634 |
| C | 4.50259 | 16.66842 | 4.06624 |
| C | 10.13568 | 19.09618 | 4.44736 |
| C | 9.98114 | 20.21981 | 5.49122 |
| C | 7.90012 | 15.22611 | 0.33301 |
| C | 7.44580 | 16.56904 | 0.93464 |
| C | 5.66182 | 10.81070 | 1.58911 |
| C | 5.86693 | 10.37585 | 0.12472 |
| C | 11.13647 | 9.56172 | 1.20251 |
| C | 12.26792 | 10.57941 | 0.95679 |
| C | 10.58293 | 7.10692 | 5.64423 |
| C | 10.22656 | 7.29556 | 7.12365 |
| C | 15.11814 | 10.90271 | 5.90482 |
| C | 14.72271 | 9.90932 | 4.79599 |
| C | 12.90111 | 10.75030 | 10.50874 |
| C | 13.03760 | 9.21985 | 10.63541 |
| C | 14.71847 | 15.43389 | 8.15546 |
| C | 14.15499 | 17.79539 | 8.71562 |
| C | 7.57074 | 17.09603 | 9.94268 |
| C | 9.28937 | 17.10572 | 11.74649 |
| C | 11.62287 | 8.18813 | 0.72043 |
| C | 9.90592 | 9.95855 | 0.36574 |
| C | 12.02124 | 6.55805 | 5.56882 |

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| C | 9.61129 | 6.07165 | 5.04360 |
| C | 9.40780 | 15.29141 | 0.01738 |
| C | 7.14809 | 15.01439 | -0.98809 |
| C | 5.87357 | 9.57143 | 2.47001 |
| C | 4.21009 | 11.30372 | 1.75560 |
| C | 4.97214 | 19.06953 | 4.51129 |
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| C | 9.88379 | 19.67107 | 3.03979 |
| C | 16.31718 | 10.31887 | 6.66474 |
| C | 15.56293 | 12.23127 | 5.26181 |
| C | 14.12578 | 11.42086 | 11.16095 |
| C | 11.65123 | 11.18987 | 11.28325 |
| C | 5.98184 | 5.94931 | 12.08877 |
| C | 6.83359 | 4.95622 | 11.52967 |
| C | 8.22086 | 4.98749 | 11.76620 |
| C | 9.04895 | 4.01459 | 11.21804 |
| C | 8.51301 | 2.99712 | 10.42777 |
| C | 7.13912 | 2.95730 | 10.18737 |
| C | 6.30295 | 3.92575 | 10.73099 |
| C | 5.25242 | 6.79719 | 12.56990 |
| C | 4.39912 | 7.78533 | 13.13545 |
| C | 4.92933 | 8.81554 | 13.93477 |
| C | 4.09134 | 9.77877 | 14.48519 |
| C | 2.71651 | 9.73341 | 14.25089 |
| C | 2.18133 | 8.71593 | 13.46031 |
| C | 3.01107 | 7.74841 | 12.90539 |
| H | 5.99929 | 8.84716 | 14.11523 |
| H | 4.51278 | 10.56861 | 15.10078 |
| H | 2.06514 | 10.48796 | 14.68272 |
| H | 1.11154 | 8.67640 | 13.27491 |
| H | 2.59866 | 6.95534 | 12.28941 |
| H | 8.63398 | 5.78038 | 12.38192 |
| H | 10.11791 | 4.04968 | 11.40925 |
| H | 9.16299 | 2.23787 | 10.00202 |
| H | 6.71687 | 2.16654 | 9.57343 |
| H | 5.23345 | 3.89772 | 10.54681 |
| H | 5.52042 | 8.99742 | 5.77143 |
| H | 7.25372 | 9.03902 | 6.08662 |
| H | 6.18958 | 8.11827 | 7.14172 |
| H | 4.76157 | 11.08502 | 5.07606 |
| H | 3.32436 | 11.09988 | 6.09671 |
| H | 4.16789 | 12.60432 | 5.73923 |
| H | 4.66312 | 14.08388 | 9.24687 |
| H | 4.00124 | 13.87220 | 7.63219 |
| H | 3.27438 | 13.01667 | 8.99714 |

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| H | 6.16393 | 13.20288 | 10.75406 |
| H | 5.43944 | 11.72659 | 11.39639 |
| H | 7.18447 | 11.81018 | 11.10838 |
| H | 8.05665 | 8.85770 | 8.82326 |
| H | 8.05291 | 9.91276 | 10.23452 |
| H | 6.80141 | 8.67581 | 10.04710 |
| H | 8.94899 | 14.94497 | 2.83491 |
| H | 7.44805 | 14.08545 | -1.48497 |
| H | 6.06286 | 14.99177 | -0.84143 |
| H | 7.36884 | 15.84043 | -1.67230 |
| H | 7.66627 | 17.39011 | 0.24232 |
| H | 6.36665 | 16.56436 | 1.11913 |
| H | 7.94263 | 16.78518 | 1.88444 |
| H | 9.75835 | 14.34880 | -0.41640 |
| H | 9.61072 | 16.09268 | -0.70261 |
| H | 10.00405 | 15.49052 | 0.91269 |
| H | 6.28736 | 12.98617 | 0.11358 |
| H | 3.50075 | 10.50958 | 1.49380 |
| H | 4.01221 | 11.61080 | 2.78728 |
| H | 4.00905 | 12.16387 | 1.10874 |
| H | 5.21060 | 9.52917 | -0.10528 |
| H | 5.62479 | 11.17100 | -0.58600 |
| H | 6.89949 | 10.06422 | -0.05733 |
| H | 5.21805 | 8.76101 | 2.13410 |
| H | 6.90743 | 9.21416 | 2.42224 |
| H | 5.63188 | 9.76421 | 3.51894 |
| H | 7.19113 | 11.19647 | 3.89939 |
| H | 10.32550 | 11.67711 | 2.72972 |
| H | 9.51042 | 10.93538 | 0.65880 |
| H | 10.16500 | 10.00192 | -0.69870 |
| H | 9.10441 | 9.22250 | 0.48869 |
| H | 13.16093 | 10.31977 | 1.53465 |
| H | 12.54233 | 10.59175 | -0.10439 |
| H | 11.97228 | 11.59547 | 1.23371 |
| H | 12.51161 | 7.85579 | 1.26754 |
| H | 10.84811 | 7.42065 | 0.82195 |
| H | 11.88979 | 8.24438 | -0.34019 |
| H | 11.09920 | 7.47157 | 3.02322 |
| H | 9.83866 | 5.85890 | 3.99459 |
| H | 9.67268 | 5.12717 | 5.59638 |
| H | 8.57694 | 6.42757 | 5.09569 |
| H | 10.31793 | 6.34046 | 7.65120 |
| H | 10.89132 | 8.01278 | 7.61577 |
| H | 9.19448 | 7.63813 | 7.24882 |
| H | 12.33209 | 6.36319 | 4.53805 |
| H | 12.73058 | 7.26786 | 6.00556 |

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| H | 12.09716 | 5.61567 | 6.12357 |
| H | 9.92896 | 9.69080 | 6.49326 |
| H | 12.69441 | 11.96539 | 5.22922 |
| H | 15.84989 | 12.95980 | 6.02710 |
| H | 16.42684 | 12.06784 | 4.60696 |
| H | 14.76758 | 12.67725 | 4.65733 |
| H | 13.87005 | 10.26805 | 4.21252 |
| H | 15.56231 | 9.75082 | 4.10873 |
| H | 14.44610 | 8.93942 | 5.22123 |
| H | 16.66769 | 10.99229 | 7.45430 |
| H | 16.08042 | 9.35073 | 7.11898 |
| H | 17.15060 | 10.16115 | 5.97183 |
| H | 14.80737 | 10.41014 | 8.61866 |
| H | 11.75428 | 10.90979 | 12.33738 |
| H | 11.50543 | 12.27380 | 11.23696 |
| H | 10.74377 | 10.71276 | 10.89991 |
| H | 13.10648 | 8.92707 | 11.68986 |
| H | 12.17049 | 8.71318 | 10.19876 |
| H | 13.93287 | 8.84992 | 10.12565 |
| H | 14.18084 | 11.15849 | 12.22385 |
| H | 15.06525 | 11.10823 | 10.69521 |
| H | 14.06098 | 12.51084 | 11.08479 |
| H | 10.81495 | 11.93555 | 9.05519 |
| H | 12.56025 | 14.56656 | 7.27286 |
| H | 15.21923 | 17.99928 | 8.88266 |
| H | 13.92585 | 18.02566 | 7.66986 |
| H | 13.58128 | 18.48486 | 9.34264 |
| H | 13.96621 | 14.99978 | 10.77290 |
| H | 15.25433 | 16.21603 | 10.68850 |
| H | 13.62636 | 16.68142 | 11.19822 |
| H | 14.54656 | 14.36978 | 8.34635 |
| H | 14.54785 | 15.62196 | 7.09013 |
| H | 15.77332 | 15.64491 | 8.36213 |
| H | 11.74202 | 17.49720 | 10.29276 |
| H | 10.31009 | 17.35857 | 12.04993 |
| H | 8.60221 | 17.67947 | 12.37944 |
| H | 9.13465 | 16.04146 | 11.95251 |
| H | 9.07006 | 19.17900 | 8.96279 |
| H | 8.57893 | 19.51847 | 10.63245 |
| H | 10.28178 | 19.23222 | 10.25080 |
| H | 7.32020 | 17.31702 | 8.90050 |
| H | 7.33764 | 16.04253 | 10.12788 |
| H | 6.91496 | 17.69956 | 10.57973 |
| H | 8.51711 | 15.53184 | 8.25933 |
| H | 10.54771 | 16.41285 | 5.10690 |
| H | 10.60380 | 20.46775 | 2.81933 |

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| H | 9.99151 | 18.89531 | 2.27455 |
| H | 8.87986 | 20.09586 | 2.94501 |
| H | 10.69142 | 21.03015 | 5.28889 |
| H | 8.97442 | 20.64866 | 5.48074 |
| H | 10.17501 | 19.84183 | 6.50012 |
| H | 12.27058 | 19.41477 | 4.28893 |
| H | 11.83775 | 18.19493 | 5.49304 |
| H | 11.76941 | 17.80362 | 3.76375 |
| H | 7.43438 | 19.28748 | 4.46670 |
| H | 5.24041 | 18.19642 | 7.09960 |
| H | 3.66348 | 17.68716 | 6.46756 |
| H | 4.91880 | 16.48239 | 6.81711 |
| H | 4.85322 | 16.74894 | 3.03270 |
| H | 4.62358 | 15.62705 | 4.37734 |
| H | 3.43058 | 16.89710 | 4.08093 |
| H | 5.42813 | 19.82064 | 5.16488 |
| H | 5.32951 | 19.24024 | 3.48993 |
| H | 3.89103 | 19.24466 | 4.51823 |
| H | 6.46705 | 15.24690 | 5.52270 |
| H | 6.80559 | 14.22143 | 7.53773 |
| H | 8.81896 | 12.18618 | 8.99662 |

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PhCCPh TS

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| C | 8.60446 | 11.50983 | 11.72125 |
| C | 8.50189 | 10.16474 | 11.33607 |
| C | 8.07178 | 9.21578 | 12.28549 |
| C | 7.74871 | 9.60652 | 13.57980 |
| C | 7.85336 | 10.94640 | 13.95296 |
| C | 8.28472 | 11.89016 | 13.02134 |
| C | 8.87407 | 9.65664 | 10.04332 |
| C | 9.28829 | 8.86552 | 9.20003 |
| C | 9.85564 | 7.72027 | 8.55048 |
| C | 11.08360 | 7.77946 | 7.86703 |
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| C | 11.08573 | 5.36888 | 7.62419 |
| C | 9.85251 | 5.30334 | 8.27346 |
| C | 9.24276 | 6.46322 | 8.73617 |
| Th | 7.80737 | 11.42871 | 7.17344 |
| C | 5.15491 | 11.28407 | 6.35155 |
| C | 5.04951 | 11.67372 | 7.71754 |
| C | 5.46144 | 10.57795 | 8.52403 |
| C | 5.80398 | 9.49725 | 7.65705 |
| C | 5.61331 | 9.93280 | 6.31726 |
| C | 4.41556 | 12.92293 | 8.24913 |
| C | 5.30403 | 10.51643 | 10.01447 |
| C | 6.07768 | 8.08331 | 8.07603 |

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| C | 5.68380 | 9.06367 | 5.09775 |
| C | 4.70205 | 12.08772 | 5.16691 |
| C | 9.01719 | 13.72088 | 5.86599 |
| C | 10.01422 | 13.26267 | 6.78464 |
| C | 10.51185 | 12.00288 | 6.32085 |
| C | 9.79881 | 11.66575 | 5.12019 |
| C | 8.88592 | 12.74203 | 4.82563 |
| C | 10.58414 | 14.13118 | 7.85119 |
| C | 9.76474 | 14.70350 | 8.83125 |
| C | 10.27727 | 15.60949 | 9.76493 |
| C | 11.63757 | 15.93107 | 9.68845 |
| C | 12.49322 | 15.37619 | 8.72902 |
| C | 11.94393 | 14.47201 | 7.81379 |
| C | 13.97290 | 15.79264 | 8.70172 |
| C | 14.77505 | 15.01661 | 7.64814 |
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| C | 8.54593 | 15.14075 | 5.83993 |
| C | 7.23606 | 15.55573 | 6.07158 |
| C | 6.87590 | 16.91332 | 6.01049 |
| C | 7.87018 | 17.84209 | 5.70148 |
| C | 9.20057 | 17.46731 | 5.45274 |
| C | 9.51609 | 16.11244 | 5.53067 |
| C | 8.15230 | 12.90135 | 3.53764 |
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| C | 7.52082 | 14.34199 | 1.65755 |
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| C | 7.57670 | 11.80955 | 2.85740 |
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| C | 11.21871 | 10.17843 | 1.94771 |
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| C | 11.70105 | 11.31622 | 6.89027 |
| C | 12.69877 | 10.82351 | 6.04034 |
| C | 13.88689 | 10.27017 | 6.53747 |
| C | 14.05057 | 10.21541 | 7.92214 |
| C | 13.08614 | 10.71036 | 8.81546 |
| C | 11.91386 | 11.25171 | 8.28179 |
| C | 11.92207 | 10.71955 | 0.69438 |
| C | 12.31473 | 9.60392 | -0.28367 |
| C | 9.99319 | 6.82590 | 3.36958 |
| C | 11.32946 | 6.06835 | 3.49611 |
| C | 7.53457 | 15.73485 | 1.00967 |

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| C | 8.99018 | 16.22210 | 0.87127 |
| C | 6.33086 | 10.77503 | 0.85257 |
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| C | 5.19611 | 18.83792 | 6.08054 |
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| C | 16.19021 | 9.19723 | 6.27297 |
| C | 13.35182 | 10.61998 | 10.32672 |
| C | 14.75255 | 11.17289 | 10.65501 |
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| C | 10.44145 | 19.43078 | 6.38865 |
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| C | 6.74913 | 16.71815 | 1.89749 |
| C | 4.82323 | 10.74843 | 1.17465 |
| C | 6.49844 | 10.91631 | -0.67282 |
| C | 10.97749 | 11.69262 | -0.03776 |
| C | 13.20398 | 11.47082 | 1.10267 |
| C | 9.25984 | 6.33744 | 2.10463 |
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| C | 14.61442 | 15.53631 | 10.07919 |
| C | 9.99109 | 15.95279 | 12.24018 |
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| H | 7.59918 | 11.25286 | 14.96385 |
| H | 7.41580 | 8.86229 | 14.29794 |
| H | 8.00197 | 8.17178 | 11.99505 |
| H | 11.57107 | 8.73621 | 7.72224 |
| H | 12.65474 | 6.67074 | 6.92579 |
| H | 11.56974 | 4.46041 | 7.27737 |
| H | 9.36963 | 4.34345 | 8.43439 |
| H | 8.29982 | 6.40721 | 9.26967 |
| H | 5.87725 | 9.64824 | 4.19548 |
| H | 6.46043 | 8.29631 | 5.17379 |
| H | 4.73283 | 8.53736 | 4.93733 |
| H | 5.36398 | 11.98250 | 4.30182 |
| H | 3.69691 | 11.78159 | 4.84731 |

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| H | 4.65303 | 13.15372 | 5.40139 |
| H | 4.93426 | 13.29176 | 9.13731 |
| H | 4.41860 | 13.72713 | 7.51060 |
| H | 3.36886 | 12.73370 | 8.52588 |
| H | 5.64751 | 11.43155 | 10.50344 |
| H | 4.24751 | 10.37587 | 10.28195 |
| H | 5.86206 | 9.68795 | 10.45400 |
| H | 6.76797 | 7.56900 | 7.40001 |
| H | 6.50464 | 8.03849 | 9.08053 |
| H | 5.14726 | 7.49937 | 8.08819 |
| H | 8.58274 | 14.99562 | 3.40655 |
| H | 7.42604 | 15.07210 | -1.07939 |
| H | 5.84570 | 15.44247 | -0.35934 |
| H | 6.94357 | 16.75015 | -0.80710 |
| H | 6.76612 | 17.72387 | 1.46088 |
| H | 5.70318 | 16.40557 | 1.98687 |
| H | 7.16792 | 16.78079 | 2.90560 |
| H | 9.57408 | 15.54088 | 0.24309 |
| H | 9.01571 | 17.21562 | 0.40839 |
| H | 9.48749 | 16.29370 | 1.84267 |
| H | 6.48774 | 13.36221 | 0.06032 |
| H | 4.32690 | 9.93260 | 0.63542 |
| H | 4.64781 | 10.60197 | 2.24488 |
| H | 4.34349 | 11.68888 | 0.88391 |
| H | 6.10904 | 10.02098 | -1.16969 |
| H | 5.94864 | 11.76979 | -1.07986 |
| H | 7.55127 | 11.02681 | -0.95177 |
| H | 6.51497 | 8.62517 | 0.65695 |
| H | 8.03850 | 9.42784 | 1.08570 |
| H | 6.78329 | 9.18444 | 2.30368 |
| H | 7.63532 | 10.82842 | 3.31538 |
| H | 10.99680 | 12.12839 | 2.84784 |
| H | 10.67927 | 12.53047 | 0.59862 |
| H | 11.46946 | 12.10197 | -0.92782 |
| H | 10.06401 | 11.18220 | -0.35840 |
| H | 13.90339 | 10.80460 | 1.61809 |
| H | 13.70823 | 11.87064 | 0.21539 |
| H | 12.98915 | 12.31305 | 1.76745 |
| H | 13.00538 | 8.88584 | 0.17165 |
| H | 11.44055 | 9.05510 | -0.64998 |
| H | 12.81738 | 10.03761 | -1.15452 |
| H | 11.23625 | 8.11529 | 1.36560 |
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| H | 8.30721 | 6.85988 | 1.97499 |
| H | 8.93507 | 5.39762 | 4.60295 |

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| H | 8.14133 | 6.97268 | 4.51574 |
| H | 11.98236 | 6.25932 | 2.63862 |
| H | 11.86448 | 6.37109 | 4.40064 |
| H | 11.15219 | 4.98772 | 3.54951 |
| H | 9.42037 | 8.90305 | 5.16497 |
| H | 12.55369 | 10.90536 | 4.96944 |
| H | 15.87887 | 11.79451 | 5.40680 |
| H | 16.24642 | 10.72567 | 4.03967 |
| H | 14.65084 | 11.48040 | 4.17374 |
| H | 13.53992 | 9.12000 | 4.04036 |
| H | 15.17033 | 8.45182 | 3.86577 |
| H | 14.09616 | 7.85324 | 5.13889 |
| H | 16.68290 | 9.91864 | 6.93328 |
| H | 15.91572 | 8.31937 | 6.86805 |
| H | 16.92835 | 8.87493 | 5.53084 |
| H | 14.95990 | 9.78766 | 8.32829 |
| H | 12.57777 | 11.36962 | 12.20390 |
| H | 12.31023 | 12.47413 | 10.84461 |
| H | 11.31712 | 11.01615 | 11.02542 |
| H | 13.49170 | 9.05546 | 11.83841 |
| H | 12.29292 | 8.72272 | 10.57504 |
| H | 14.01830 | 8.53151 | 10.23031 |
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| H | 15.55272 | 10.59130 | 10.18750 |
| H | 14.85569 | 12.21037 | 10.32278 |
| H | 11.14453 | 11.64369 | 8.93735 |
| H | 12.56463 | 14.02288 | 7.04666 |
| H | 15.12648 | 17.61527 | 8.37602 |
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| H | 15.67403 | 15.81674 | 10.06311 |
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| H | 14.40690 | 15.20768 | 6.63462 |
| H | 15.82476 | 15.32795 | 7.67952 |
| H | 12.04644 | 16.64300 | 10.40090 |
| H | 11.00496 | 16.34843 | 12.35583 |
| H | 9.36976 | 16.40192 | 13.02403 |
| H | 10.03650 | 14.87282 | 12.41570 |
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| H | 7.47267 | 15.97447 | 9.85890 |
| H | 7.90202 | 14.66814 | 10.96987 |

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| H | 8.71886 | 14.41653 | 8.84224 |
| H | 10.53095 | 15.77474 | 5.35333 |
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| H | 11.18357 | 20.21396 | 6.19266 |
| H | 9.50775 | 19.92148 | 6.68168 |
| H | 10.78780 | 18.83512 | 7.23896 |
| H | 12.31967 | 18.74163 | 4.53883 |
| H | 12.02534 | 17.34123 | 5.57623 |
| H | 11.53319 | 17.30470 | 3.87315 |
| H | 7.61223 | 18.89438 | 5.65545 |
| H | 5.78082 | 17.61072 | 8.45633 |
| H | 4.08698 | 17.29614 | 8.03629 |
| H | 5.26730 | 15.97441 | 8.02743 |
| H | 4.63903 | 16.76541 | 4.36285 |
| H | 4.52418 | 15.48293 | 5.57183 |
| H | 3.41689 | 16.85751 | 5.64536 |
| H | 5.81303 | 19.46013 | 6.73744 |
| H | 5.40132 | 19.12394 | 5.04316 |
| H | 4.14926 | 19.08222 | 6.29040 |
| H | 6.50366 | 14.80228 | 6.34011 |
| H | 7.09171 | 13.23455 | 7.64805 |
| H | 8.29282 | 11.89146 | 9.11704 |

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| C | 8.24981 | 10.74717 | 9.91799 |
| C | 8.27961 | 10.76991 | 11.39472 |
| C | 7.50633 | 11.73245 | 12.06636 |
| H | 6.91198 | 12.43227 | 11.48310 |
| C | 7.48525 | 11.80114 | 13.45619 |
| H | 6.87433 | 12.55194 | 13.94994 |
| C | 8.25038 | 10.91233 | 14.20965 |
| H | 8.23999 | 10.96366 | 15.29485 |
| C | 9.03587 | 9.96108 | 13.55792 |
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| C | 9.10730 | 8.49586 | 9.17383 |
| C | 10.27205 | 8.05054 | 8.52323 |
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| C | 10.73770 | 6.74762 | 8.69648 |
| H | 11.65513 | 6.44023 | 8.20143 |
| C | 10.03398 | 5.84166 | 9.48838 |

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| H | 10.39191 | 4.82318 | 9.61054 |
| C | 8.86373 | 6.25951 | 10.12240 |
| H | 8.30239 | 5.56588 | 10.74345 |
| C | 8.41339 | 7.56790 | 9.97589 |
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| C | 5.19913 | 11.43510 | 6.09667 |
| C | 4.93424 | 11.64306 | 7.48217 |
| C | 5.24140 | 10.43702 | 8.17563 |
| C | 5.70550 | 9.48567 | 7.22886 |
| C | 5.89004 | 9.36410 | 4.65509 |
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| H | 6.85392 | 8.84414 | 4.60648 |
| H | 5.11198 | 8.60126 | 4.52001 |
| C | 4.85023 | 12.39113 | 4.99215 |
| H | 5.39745 | 12.17941 | 4.07095 |
| H | 3.77789 | 12.33860 | 4.76135 |
| H | 5.06885 | 13.42981 | 5.25635 |
| C | 4.22266 | 12.82517 | 8.06959 |
| H | 4.53784 | 13.02732 | 9.09604 |
| H | 4.39994 | 13.73409 | 7.49091 |
| H | 3.13691 | 12.65560 | 8.08147 |
| C | 4.94811 | 10.17209 | 9.62217 |
| H | 5.00441 | 11.08269 | 10.22427 |
| H | 3.93405 | 9.76811 | 9.74237 |
| H | 5.64248 | 9.45067 | 10.05936 |
| C | 5.95524 | 8.02555 | 7.46439 |
| H | 6.85175 | 7.65866 | 6.95510 |
| H | 6.07574 | 7.79762 | 8.52424 |
| H | 5.10941 | 7.43001 | 7.09392 |
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| C | 9.81968 | 11.63336 | 5.27578 |
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| C | 10.01259 | 13.23311 | 6.93220 |
| C | 9.04957 | 13.70155 | 5.98589 |
| C | 8.23128 | 12.89608 | 3.63116 |
| C | 8.05077 | 14.18035 | 3.09978 |
| H | 8.40735 | 15.03164 | 3.66353 |
| C | 7.44771 | 14.39896 | 1.85476 |
| C | 7.31029 | 15.83133 | 1.31790 |
| C | 6.63386 | 15.87961 | -0.05937 |
| H | 7.20456 | 15.33041 | -0.81600 |
| H | 5.61824 | 15.47025 | -0.02999 |
| H | 6.55908 | 16.91955 | -0.39479 |
| C | 6.46751 | 16.67248 | 2.29446 |
| H | 6.36849 | 17.69954 | 1.92346 |

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| H | 5.46175 | 16.25150 | 2.39875 |
| H | 6.91837 | 16.71824 | 3.28955 |
| C | 8.71304 | 16.45560 | 1.18364 |
| H | 9.33525 | 15.87692 | 0.49251 |
| H | 8.63993 | 17.47964 | 0.79872 |
| H | 9.22916 | 16.49526 | 2.14731 |
| C | 7.02416 | 13.28827 | 1.12889 |
| H | 6.55137 | 13.43656 | 0.16577 |
| C | 7.21142 | 11.97784 | 1.59260 |
| C | 6.74035 | 10.80789 | 0.70916 |
| C | 5.20241 | 10.71524 | 0.77113 |
| H | 4.83976 | 9.90613 | 0.12602 |
| H | 4.85224 | 10.51616 | 1.78878 |
| H | 4.73663 | 11.64818 | 0.43708 |
| C | 7.15095 | 11.03835 | -0.75995 |
| H | 6.87108 | 10.16784 | -1.36378 |
| H | 6.65728 | 11.90785 | -1.20294 |
| H | 8.23120 | 11.18322 | -0.85359 |
| C | 7.34546 | 9.46651 | 1.14557 |
| H | 7.03893 | 8.67976 | 0.44769 |
| H | 8.43909 | 9.50311 | 1.15746 |
| H | 7.01160 | 9.16244 | 2.14031 |
| C | 7.80537 | 11.80117 | 2.84642 |
| H | 7.96672 | 10.79890 | 3.22224 |
| C | 10.21897 | 10.54146 | 4.33802 |
| C | 10.91095 | 10.90524 | 3.17744 |
| H | 11.09490 | 11.96176 | 3.00465 |
| C | 11.37106 | 9.95283 | 2.25906 |
| C | 12.15475 | 10.40528 | 1.01681 |
| C | 11.26705 | 11.32399 | 0.15673 |
| H | 10.91548 | 12.19542 | 0.71608 |
| H | 11.82539 | 11.68424 | -0.71503 |
| H | 10.38713 | 10.78343 | -0.20485 |
| C | 13.41161 | 11.18283 | 1.45267 |
| H | 14.07674 | 10.55160 | 2.05028 |
| H | 13.96913 | 11.52422 | 0.57290 |
| H | 13.16045 | 12.06621 | 2.04763 |
| C | 12.60630 | 9.22392 | 0.14670 |
| H | 13.26712 | 8.54299 | 0.69362 |
| H | 11.75648 | 8.64773 | -0.23470 |
| H | 13.16253 | 9.59791 | -0.71926 |
| C | 11.08601 | 8.61117 | 2.52526 |
| H | 11.42591 | 7.85303 | 1.82862 |
| C | 10.37420 | 8.19833 | 3.66288 |
| C | 10.08760 | 6.70036 | 3.85501 |
| C | 9.36412 | 6.14651 | 2.61079 |

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| H | 9.96569 | 6.24569 | 1.70251 |
| H | 9.14590 | 5.08112 | 2.74673 |
| H | 8.41636 | 6.66779 | 2.44250 |
| C | 9.19986 | 6.42184 | 5.07378 |
| H | 9.01646 | 5.34533 | 5.15617 |
| H | 9.66058 | 6.74539 | 6.01150 |
| H | 8.22459 | 6.91167 | 4.98108 |
| C | 11.41798 | 5.94507 | 4.04235 |
| H | 12.08544 | 6.07905 | 3.18534 |
| H | 11.94466 | 6.29770 | 4.93420 |
| H | 11.23222 | 4.87104 | 4.15818 |
| C | 9.96337 | 9.18101 | 4.57065 |
| H | 9.44164 | 8.89274 | 5.47875 |
| C | 11.68120 | 11.27595 | 7.10041 |
| C | 12.69041 | 10.74406 | 6.28799 |
| H | 12.57204 | 10.78873 | 5.21191 |
| C | 13.85987 | 10.18988 | 6.82869 |
| C | 14.95600 | 9.66035 | 5.89238 |
| C | 15.48446 | 10.82405 | 5.03086 |
| H | 15.91329 | 11.61141 | 5.65975 |
| H | 16.26655 | 10.47216 | 4.34747 |
| H | 14.69057 | 11.27442 | 4.42846 |
| C | 14.37668 | 8.56485 | 4.97906 |
| H | 13.53607 | 8.92739 | 4.38092 |
| H | 15.14638 | 8.19535 | 4.29102 |
| H | 14.02034 | 7.71604 | 5.57222 |
| C | 16.14439 | 9.05987 | 6.65730 |
| H | 16.64118 | 9.80178 | 7.29149 |
| H | 15.84096 | 8.21737 | 7.28826 |
| H | 16.88821 | 8.68688 | 5.94507 |
| C | 14.00091 | 10.18623 | 8.21560 |
| H | 14.89673 | 9.76050 | 8.65167 |
| C | 13.03057 | 10.73101 | 9.07074 |
| C | 13.26237 | 10.70186 | 10.58991 |
| C | 12.30714 | 11.64557 | 11.33325 |
| H | 12.54559 | 11.64573 | 12.40237 |
| H | 12.39244 | 12.67393 | 10.96718 |
| H | 11.26331 | 11.33610 | 11.23884 |
| C | 13.04700 | 9.26249 | 11.09737 |
| H | 13.19545 | 9.21033 | 12.18268 |
| H | 12.03630 | 8.91189 | 10.86939 |
| H | 13.75035 | 8.56706 | 10.62703 |
| C | 14.70275 | 11.13303 | 10.92803 |
| H | 14.83601 | 11.16318 | 12.01520 |
| H | 15.45239 | 10.44240 | 10.53058 |
| H | 14.92167 | 12.12956 | 10.53249 |

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| C | 11.87427 | 11.25952 | 8.49559 |
| H | 11.10089 | 11.68091 | 9.12584 |
| C | 10.60723 | 14.10088 | 7.98784 |
| C | 11.96584 | 14.43740 | 7.88793 |
| H | 12.54562 | 13.99268 | 7.08716 |
| C | 12.56440 | 15.32539 | 8.78543 |
| C | 14.04183 | 15.73783 | 8.68792 |
| C | 14.13415 | 17.24690 | 8.38802 |
| H | 15.18270 | 17.56304 | 8.33578 |
| H | 13.66074 | 17.48794 | 7.43095 |
| H | 13.64349 | 17.84439 | 9.16278 |
| C | 14.75308 | 15.45232 | 10.02454 |
| H | 14.70077 | 14.38926 | 10.27725 |
| H | 15.80996 | 15.73606 | 9.96083 |
| H | 14.31012 | 16.01316 | 10.85291 |
| C | 14.78534 | 14.97851 | 7.58058 |
| H | 14.75511 | 13.89590 | 7.74078 |
| H | 14.36781 | 15.18899 | 6.59025 |
| H | 15.83648 | 15.28600 | 7.56438 |
| C | 11.76120 | 15.86465 | 9.79844 |
| H | 12.20943 | 16.56139 | 10.50201 |
| C | 10.40676 | 15.54559 | 9.94106 |
| C | 9.59854 | 16.18394 | 11.08062 |
| C | 10.26323 | 15.86632 | 12.43434 |
| H | 11.28408 | 16.25615 | 12.49265 |
| H | 9.69010 | 16.31736 | 13.25290 |
| H | 10.30641 | 14.78586 | 12.60483 |
| C | 9.55507 | 17.71133 | 10.87789 |
| H | 9.08436 | 17.96376 | 9.92227 |
| H | 8.97876 | 18.18723 | 11.68020 |
| H | 10.55759 | 18.15073 | 10.88259 |
| C | 8.15700 | 15.66367 | 11.12853 |
| H | 7.61324 | 15.87889 | 10.20416 |
| H | 8.12830 | 14.58289 | 11.29722 |
| H | 7.61835 | 16.14456 | 11.95252 |
| C | 9.84063 | 14.66004 | 9.01590 |
| H | 8.79003 | 14.39372 | 9.06922 |
| C | 8.57004 | 15.11908 | 6.01045 |
| C | 9.51082 | 16.10471 | 5.65846 |
| H | 10.50570 | 15.77617 | 5.38031 |
| C | 9.19284 | 17.46072 | 5.67098 |
| C | 10.21353 | 18.55461 | 5.32509 |
| C | 9.64764 | 19.48956 | 4.23884 |
| H | 10.37510 | 20.27435 | 4.00192 |
| H | 9.43122 | 18.93879 | 3.31800 |
| H | 8.72491 | 19.98283 | 4.55815 |

| | | | |
|---|---|---|---|
| C | 10.51178 | 19.37507 | 6.59603 |
| H | 11.23952 | 20.16610 | 6.37939 |
| H | 9.60769 | 19.85119 | 6.98851 |
| H | 10.92309 | 18.73637 | 7.38387 |
| C | 11.53439 | 17.97099 | 4.80557 |
| H | 12.22603 | 18.78356 | 4.55883 |
| H | 12.02121 | 17.33784 | 5.55375 |
| H | 11.38624 | 17.37542 | 3.89816 |
| C | 7.89105 | 17.82154 | 6.05600 |
| H | 7.63448 | 18.87462 | 6.08213 |
| C | 6.92667 | 16.88020 | 6.41574 |
| C | 5.51368 | 17.29243 | 6.85852 |
| C | 5.27705 | 16.82695 | 8.30804 |
| H | 5.97239 | 17.32417 | 8.99218 |
| H | 4.25683 | 17.07177 | 8.62675 |
| H | 5.41509 | 15.74797 | 8.41960 |
| C | 4.46775 | 16.64421 | 5.93227 |
| H | 4.60330 | 16.97367 | 4.89733 |
| H | 4.53169 | 15.55286 | 5.94395 |
| H | 3.45518 | 16.92079 | 6.24807 |
| C | 5.30067 | 18.81244 | 6.81113 |
| H | 5.98484 | 19.34319 | 7.48166 |
| H | 5.42911 | 19.21218 | 5.79954 |
| H | 4.28031 | 19.04785 | 7.13172 |
| C | 7.28877 | 15.52056 | 6.38419 |
| H | 6.57878 | 14.75979 | 6.69450 |
| Th | 7.74129 | 11.42587 | 7.25967 |
| H | 7.14806 | 13.09888 | 8.29958 |
| H | 7.79648 | 11.72418 | 9.58456 |

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PhCCCCPh

| | | | |
|---|---|---|---|
| C | 2.98794 | 7.75740 | 12.91935 |
| C | 4.37629 | 7.79872 | 13.15247 |
| C | 4.90461 | 8.83041 | 13.95248 |
| C | 4.06326 | 9.79091 | 14.50117 |
| C | 2.68892 | 9.74170 | 14.26455 |
| C | 2.15619 | 8.72330 | 13.47318 |
| C | 5.23048 | 6.81513 | 12.58976 |
| C | 5.96643 | 5.96799 | 12.10529 |
| C | 8.37451 | 3.19660 | 10.52025 |
| C | 9.76264 | 3.23745 | 10.75469 |
| C | 10.59469 | 2.27167 | 10.20109 |
| C | 10.06246 | 1.25383 | 9.40867 |
| C | 8.68832 | 1.20507 | 9.17075 |
| C | 7.84668 | 2.16546 | 9.71919 |
| H | 5.97438 | 8.86395 | 14.13331 |

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|---|---|---|---|
| H | 4.48151 | 10.58237 | 15.11674 |
| H | 2.03516 | 10.49462 | 14.69557 |
| H | 1.08673 | 8.68165 | 13.28675 |
| H | 2.57901 | 6.96286 | 12.30314 |
| H | 10.17119 | 4.03156 | 11.37172 |
| H | 11.66398 | 2.31297 | 10.38854 |
| H | 10.71643 | 0.50097 | 8.97788 |
| H | 8.27045 | 0.41404 | 8.55438 |
| H | 6.77708 | 2.13227 | 9.53736 |
| C | 6.78392 | 5.02709 | 11.56716 |
| C | 7.52002 | 4.18004 | 11.08276 |

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PhCCCCPh adduct

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| C | 4.93240 | 9.34890 | 13.68898 |
| C | 4.44359 | 8.26274 | 12.93736 |
| C | 3.05215 | 8.06966 | 12.83906 |
| C | 2.17819 | 8.94203 | 13.47687 |
| C | 2.67160 | 10.01565 | 14.21911 |
| C | 4.04888 | 10.21504 | 14.32217 |
| C | 5.34151 | 7.37599 | 12.28802 |
| C | 6.11693 | 6.61332 | 11.72985 |
| C | 6.97962 | 5.76847 | 11.10899 |
| C | 7.75787 | 5.01100 | 10.54826 |
| C | 8.66388 | 4.13631 | 9.89418 |
| C | 10.05412 | 4.33175 | 10.00947 |
| C | 10.93729 | 3.47396 | 9.36402 |
| C | 10.45470 | 2.41250 | 8.59728 |
| C | 9.07912 | 2.21049 | 8.47820 |
| C | 8.18663 | 3.06184 | 9.11891 |
| C | 7.57094 | 9.95757 | 9.12761 |
| C | 6.72099 | 10.95053 | 8.39177 |
| C | 6.19152 | 12.15709 | 8.92662 |
| C | 5.35310 | 12.75176 | 7.93964 |
| C | 5.36317 | 11.90879 | 6.78977 |
| C | 6.21488 | 10.79586 | 7.06733 |
| Th | 7.94990 | 12.95624 | 6.84051 |
| C | 9.11870 | 13.68366 | 4.39187 |
| C | 9.97603 | 12.65481 | 4.90699 |
| C | 10.67454 | 13.18190 | 6.04221 |
| C | 10.23695 | 14.52707 | 6.23873 |
| C | 9.27799 | 14.84107 | 5.22404 |
| C | 10.26525 | 11.33720 | 4.28471 |
| C | 10.33246 | 10.16283 | 5.05576 |
| C | 10.68749 | 8.93750 | 4.48819 |
| C | 10.99102 | 8.91295 | 3.11783 |
| C | 10.95262 | 10.05697 | 2.31857 |

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| C | 10.57166 | 11.26309 | 2.92264 |
| C | 11.32589 | 10.03867 | 0.82839 |
| C | 12.46755 | 11.04168 | 0.56989 |
| C | 10.77600 | 7.63441 | 5.29762 |
| C | 10.44119 | 7.84229 | 6.77955 |
| C | 11.84905 | 12.53020 | 6.69208 |
| C | 11.90763 | 12.23696 | 8.06232 |
| C | 13.04342 | 11.65505 | 8.62832 |
| C | 14.13893 | 11.38713 | 7.79163 |
| C | 14.12778 | 11.68174 | 6.42675 |
| C | 12.96174 | 12.24788 | 5.89344 |
| C | 10.72021 | 15.47744 | 7.26997 |
| C | 9.80715 | 16.22739 | 8.02394 |
| C | 10.24151 | 17.14836 | 8.98155 |
| C | 11.62088 | 17.31401 | 9.14871 |
| C | 12.56565 | 16.59309 | 8.40830 |
| C | 12.09384 | 15.66805 | 7.47268 |
| C | 8.78738 | 16.21552 | 4.92101 |
| C | 7.43701 | 16.55438 | 4.85030 |
| C | 7.02066 | 17.85473 | 4.52906 |
| C | 8.00570 | 18.80836 | 4.26551 |
| C | 9.37719 | 18.50900 | 4.31753 |
| C | 9.74681 | 17.20586 | 4.64792 |
| C | 8.35430 | 13.62975 | 3.11675 |
| C | 8.54071 | 14.64803 | 2.17522 |
| C | 7.90387 | 14.62670 | 0.92862 |
| C | 7.05144 | 13.55655 | 0.65159 |
| C | 6.84119 | 12.50430 | 1.55579 |
| C | 7.50587 | 12.55777 | 2.78541 |
| C | 6.40520 | 12.67423 | 10.31777 |
| C | 6.43767 | 9.59479 | 6.18704 |
| C | 4.51208 | 12.10477 | 5.56798 |
| C | 4.45359 | 13.93424 | 8.15211 |
| C | 13.11980 | 11.28143 | 10.11665 |
| C | 13.25499 | 9.75103 | 10.24559 |
| C | 15.33219 | 11.41909 | 5.50979 |
| C | 14.93323 | 10.41656 | 4.41042 |
| C | 9.26810 | 17.96938 | 9.83971 |
| C | 9.49788 | 19.47229 | 9.58602 |
| C | 14.06321 | 16.84585 | 8.63971 |
| C | 14.41180 | 16.56371 | 10.11424 |
| C | 5.52196 | 18.19153 | 4.52655 |
| C | 4.75864 | 17.21316 | 3.61388 |
| C | 10.40606 | 19.61140 | 4.02542 |
| C | 10.25258 | 20.73915 | 5.06503 |
| C | 8.18155 | 15.74674 | -0.08489 |

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| C | 7.74117 | 17.09860 | 0.50702 |
| C | 5.87177 | 11.37119 | 1.17969 |
| C | 6.07130 | 10.93171 | -0.28406 |
| C | 14.34535 | 11.95185 | 10.76732 |
| C | 11.87047 | 11.72301 | 10.89093 |
| C | 16.53352 | 10.84156 | 6.27093 |
| C | 15.77509 | 12.74231 | 4.85467 |
| C | 7.80177 | 17.65062 | 9.52065 |
| C | 9.51505 | 17.66075 | 11.32951 |
| C | 14.94757 | 15.95149 | 7.76038 |
| C | 14.39240 | 18.31622 | 8.31477 |
| C | 5.24237 | 19.61675 | 4.02897 |
| C | 4.98446 | 18.06556 | 5.96607 |
| C | 11.84954 | 19.09389 | 4.09335 |
| C | 10.16835 | 20.18420 | 2.61456 |
| C | 9.69185 | 15.79055 | -0.39147 |
| C | 7.43488 | 15.53799 | -1.40949 |
| C | 6.06508 | 10.13032 | 2.06235 |
| C | 4.42747 | 11.88586 | 1.34515 |
| C | 11.79577 | 8.65532 | 0.35798 |
| C | 10.09747 | 10.44098 | -0.00888 |
| C | 12.20727 | 7.06887 | 5.21059 |
| C | 9.78623 | 6.60320 | 4.71990 |
| H | 6.00461 | 9.49909 | 13.76593 |
| H | 4.43643 | 11.04985 | 14.89926 |
| H | 1.98484 | 10.69525 | 14.71565 |
| H | 1.10655 | 8.78411 | 13.39433 |
| H | 2.67402 | 7.23317 | 12.25984 |
| H | 10.42383 | 5.15789 | 10.60866 |
| H | 12.00755 | 3.63326 | 9.46107 |
| H | 11.14848 | 1.74409 | 8.09532 |
| H | 8.69991 | 1.38444 | 7.88315 |
| H | 7.11569 | 2.90906 | 9.02968 |
| H | 5.79113 | 9.62451 | 5.30630 |
| H | 7.46936 | 9.49236 | 5.82387 |
| H | 6.20243 | 8.67036 | 6.72705 |
| H | 4.94751 | 11.64073 | 4.67891 |
| H | 3.51490 | 11.66571 | 5.70469 |
| H | 4.36410 | 13.16519 | 5.33945 |
| H | 4.90000 | 14.66791 | 8.82751 |
| H | 4.23293 | 14.45293 | 7.21569 |
| H | 3.49507 | 13.62010 | 8.58829 |
| H | 6.37773 | 13.76784 | 10.35128 |
| H | 5.62491 | 12.30895 | 10.99881 |
| H | 7.37211 | 12.35895 | 10.71787 |
| H | 8.19217 | 9.36691 | 8.44820 |

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| H | 8.24020 | 10.45049 | 9.83767 |
| H | 6.95053 | 9.24836 | 9.69108 |
| H | 9.21195 | 15.46278 | 2.42533 |
| H | 7.72588 | 14.60281 | -1.89995 |
| H | 6.34860 | 15.52998 | -1.26927 |
| H | 7.67027 | 16.35772 | -2.09638 |
| H | 7.97743 | 17.91307 | -0.18788 |
| H | 6.66081 | 17.10950 | 0.68403 |
| H | 8.23423 | 17.31292 | 1.45919 |
| H | 10.03281 | 14.84089 | -0.81743 |
| H | 9.90955 | 16.58473 | -1.11497 |
| H | 10.28515 | 15.98740 | 0.50631 |
| H | 6.53893 | 13.52883 | -0.30239 |
| H | 3.70642 | 11.10235 | 1.08337 |
| H | 4.23386 | 12.19638 | 2.37662 |
| H | 4.23983 | 12.74857 | 0.69765 |
| H | 5.40505 | 10.09235 | -0.51220 |
| H | 5.83772 | 11.72823 | -0.99613 |
| H | 7.10007 | 10.60772 | -0.46609 |
| H | 5.39918 | 9.32832 | 1.72683 |
| H | 7.09407 | 9.75891 | 2.01764 |
| H | 5.82351 | 10.32876 | 3.11019 |
| H | 7.39516 | 11.74337 | 3.49600 |
| H | 10.53458 | 12.17562 | 2.33629 |
| H | 9.71421 | 11.42544 | 0.27482 |
| H | 10.35403 | 10.47031 | -1.07442 |
| H | 9.28773 | 9.71570 | 0.12393 |
| H | 13.35904 | 10.77870 | 1.14860 |
| H | 12.73983 | 11.04036 | -0.49195 |
| H | 12.18300 | 12.06352 | 0.83704 |
| H | 12.68318 | 8.31896 | 0.90479 |
| H | 11.01342 | 7.89711 | 0.47025 |
| H | 12.05902 | 8.69849 | -0.70416 |
| H | 11.28056 | 7.96819 | 2.67126 |
| H | 9.99979 | 6.37644 | 3.67081 |
| H | 9.84293 | 5.66486 | 5.28326 |
| H | 8.75667 | 6.97161 | 4.77905 |
| H | 10.53149 | 6.89215 | 7.31585 |
| H | 11.11808 | 8.56000 | 7.25427 |
| H | 9.41384 | 8.19480 | 6.91547 |
| H | 12.50324 | 6.85789 | 4.17860 |
| H | 12.92999 | 7.77569 | 5.63001 |
| H | 12.27878 | 6.13242 | 5.77571 |
| H | 10.14054 | 10.23116 | 6.12270 |
| H | 12.91042 | 12.48631 | 4.83494 |
| H | 16.06366 | 13.47734 | 5.61311 |

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| H | 16.63751 | 12.57352 | 4.19924 |
| H | 14.97844 | 13.18311 | 4.24810 |
| H | 14.07885 | 10.77076 | 3.82665 |
| H | 15.77064 | 10.25180 | 3.72192 |
| H | 14.65744 | 9.45043 | 4.84477 |
| H | 16.88449 | 11.52030 | 7.05573 |
| H | 16.29907 | 9.87586 | 6.73149 |
| H | 17.36580 | 10.68073 | 5.57737 |
| H | 15.02439 | 10.93528 | 8.22564 |
| H | 11.97369 | 11.44442 | 11.94540 |
| H | 11.72544 | 12.80699 | 10.84307 |
| H | 10.96263 | 11.24556 | 10.50896 |
| H | 13.32352 | 9.45989 | 11.30048 |
| H | 12.38725 | 9.24464 | 9.80993 |
| H | 14.14996 | 9.37963 | 9.73630 |
| H | 14.40071 | 11.69075 | 11.83049 |
| H | 15.28435 | 11.63790 | 10.30146 |
| H | 14.28140 | 13.04180 | 10.68987 |
| H | 11.03454 | 12.46750 | 8.66234 |
| H | 12.78827 | 15.08748 | 6.87732 |
| H | 15.45712 | 18.51566 | 8.48394 |
| H | 14.16671 | 18.54573 | 7.26810 |
| H | 13.82038 | 19.00932 | 8.93931 |
| H | 14.18634 | 15.52522 | 10.37667 |
| H | 15.47934 | 16.73638 | 10.29386 |
| H | 13.85163 | 17.20891 | 10.79783 |
| H | 14.77160 | 14.88839 | 7.95317 |
| H | 14.77995 | 16.13791 | 6.69426 |
| H | 16.00270 | 16.15925 | 7.96894 |
| H | 11.97380 | 18.03400 | 9.88268 |
| H | 10.53584 | 17.91071 | 11.63513 |
| H | 8.82831 | 18.23999 | 11.95790 |
| H | 9.35528 | 16.59804 | 11.53962 |
| H | 9.31282 | 19.72321 | 8.53649 |
| H | 8.81839 | 20.07172 | 10.20331 |
| H | 10.52108 | 19.77658 | 9.82776 |
| H | 7.55479 | 17.86894 | 8.47707 |
| H | 7.56392 | 16.59873 | 9.70894 |
| H | 7.14670 | 18.25901 | 10.15379 |
| H | 8.74632 | 16.07799 | 7.84386 |
| H | 10.79351 | 16.92942 | 4.70462 |
| H | 10.89626 | 20.97444 | 2.39692 |
| H | 10.27513 | 19.40550 | 1.85218 |
| H | 9.16865 | 20.61695 | 2.51157 |
| H | 10.97028 | 21.54364 | 4.86559 |
| H | 9.24911 | 21.17531 | 5.04604 |

H 10.43632 20.36256 6.07633
H 12.54427 19.91308 3.87889
H 12.09488 18.70201 5.08567
H 12.03395 18.30347 3.35773
H 7.70607 19.82081 4.01731
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H 5.15068 17.06244 6.37026
H 5.11978 17.27461 2.58264
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234
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C 9.12993 17.46623 5.58966
C 9.47862 16.11928 5.67367
C 10.58491 14.05728 7.86333
C 9.78028 14.71619 8.80220
C 10.32592 15.61816 9.72060
C 11.70802 15.83785 9.68125
C 12.54913 15.19900 8.76260
C 11.96477 14.30952 7.85472
Th 7.78090 11.38476 7.19371
C 5.75055 9.76163 6.21767
C 5.13958 11.03108 6.43295
C 5.03837 11.23285 7.84102

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| C | 5.59098 | 10.09766 | 8.48996 |
| C | 6.04864 | 9.19128 | 7.48672 |
| C | 4.58169 | 11.93618 | 5.37257 |
| C | 4.33431 | 12.35660 | 8.53967 |
| C | 5.46912 | 9.80714 | 9.95538 |
| C | 6.51967 | 7.78194 | 7.70245 |
| C | 5.90512 | 9.05702 | 4.90076 |
| C | 10.07248 | 10.61192 | 4.07884 |
| C | 10.65560 | 11.05498 | 2.88616 |
| C | 11.02066 | 10.17124 | 1.86339 |
| C | 10.75821 | 8.81449 | 2.06171 |
| C | 10.16286 | 8.32136 | 3.23315 |
| C | 9.84178 | 9.23658 | 4.24248 |
| C | 8.13708 | 12.96807 | 3.53793 |
| C | 8.28217 | 14.20546 | 2.89375 |
| C | 7.76496 | 14.44168 | 1.61624 |
| C | 7.08207 | 13.40035 | 0.98347 |
| C | 6.90945 | 12.14550 | 1.58022 |
| C | 7.44048 | 11.95109 | 2.86246 |
| C | 9.47321 | 16.36149 | 10.76021 |
| C | 9.65621 | 17.88290 | 10.59423 |
| C | 14.05430 | 15.51161 | 8.76839 |
| C | 14.63703 | 15.24626 | 10.17035 |
| C | 5.29895 | 17.19954 | 6.09154 |
| C | 4.46325 | 16.47892 | 5.01647 |
| C | 10.16535 | 18.57993 | 5.37149 |
| C | 10.20658 | 19.48534 | 6.61793 |
| C | 7.96455 | 15.81267 | 0.95295 |
| C | 7.18785 | 16.87498 | 1.75381 |
| C | 6.13280 | 11.03600 | 0.84888 |
| C | 6.10049 | 11.26020 | -0.67336 |
| C | 11.67448 | 10.71176 | 0.58321 |
| C | 12.95816 | 11.48382 | 0.94536 |
| C | 9.89936 | 6.81108 | 3.34208 |
| C | 9.16570 | 6.43466 | 4.63342 |
| C | 14.88582 | 9.73889 | 5.39265 |
| C | 14.29872 | 8.70250 | 4.41680 |
| C | 13.34879 | 10.39960 | 10.21620 |
| C | 13.26876 | 8.91546 | 10.62424 |
| C | 14.82906 | 14.65601 | 7.75684 |
| C | 14.27444 | 16.99571 | 8.41452 |
| C | 7.97725 | 16.05296 | 10.61459 |
| C | 9.92629 | 15.95059 | 12.17495 |
| C | 12.05333 | 9.59329 | -0.39718 |
| C | 10.69451 | 11.66473 | -0.12779 |
| C | 11.24174 | 6.05426 | 3.31242 |

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| C | 9.03159 | 6.34796 | 2.15471 |
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| C | 4.67770 | 11.02664 | 1.35770 |
| C | 5.04255 | 18.70715 | 5.95836 |
| C | 4.82717 | 16.75398 | 7.48950 |
| C | 11.57605 | 18.02323 | 5.13745 |
| C | 9.77705 | 19.42651 | 4.14384 |
| C | 16.11843 | 9.11869 | 6.06544 |
| C | 15.35022 | 10.97686 | 4.59948 |
| C | 14.76576 | 10.92076 | 10.52818 |
| C | 12.35678 | 11.20124 | 11.06915 |
| C | 8.36949 | 10.62857 | 11.57474 |
| C | 8.26624 | 12.00815 | 11.80759 |
| C | 7.90285 | 12.47559 | 13.06673 |
| C | 7.63942 | 11.58411 | 14.10634 |
| C | 7.74659 | 10.21056 | 13.88525 |
| C | 8.10964 | 9.73220 | 12.63255 |
| C | 8.77298 | 10.05610 | 10.32600 |
| C | 9.22130 | 9.22774 | 9.53058 |
| C | 11.12760 | 6.13929 | 7.87650 |
| C | 12.44582 | 6.28913 | 7.40280 |
| C | 13.16298 | 5.17551 | 6.97978 |
| C | 12.58450 | 3.90598 | 7.01748 |
| C | 11.27838 | 3.75053 | 7.48346 |
| C | 10.55099 | 4.85477 | 7.91143 |
| H | 8.45820 | 12.68463 | 10.98190 |
| H | 7.82128 | 13.54537 | 13.23468 |
| H | 7.35139 | 11.95750 | 15.08512 |
| H | 7.54549 | 9.50904 | 14.69002 |
| H | 8.19767 | 8.66472 | 12.45519 |
| H | 12.88860 | 7.28010 | 7.38011 |
| H | 14.18077 | 5.29840 | 6.62047 |
| H | 13.15051 | 3.03998 | 6.68626 |
| H | 10.82558 | 2.76358 | 7.51628 |
| H | 9.53654 | 4.73894 | 8.27993 |
| H | 5.44694 | 9.63420 | 4.09532 |
| H | 6.94774 | 8.86691 | 4.61492 |
| H | 5.40403 | 8.08132 | 4.92502 |
| H | 5.26504 | 12.08025 | 4.52929 |
| H | 3.64350 | 11.53510 | 4.96626 |
| H | 4.35942 | 12.92510 | 5.77993 |
| H | 4.85558 | 12.64820 | 9.45527 |
| H | 4.26823 | 13.24588 | 7.90980 |
| H | 3.31168 | 12.06445 | 8.81620 |

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|---|---|---|---|
| H | 5.61195 | 10.70097 | 10.56714 |
| H | 4.46870 | 9.41233 | 10.18002 |
| H | 6.19371 | 9.06121 | 10.28861 |
| H | 7.29692 | 7.48744 | 6.99050 |
| H | 6.92639 | 7.63551 | 8.70567 |
| H | 5.68819 | 7.07373 | 7.58104 |
| H | 8.83172 | 14.98965 | 3.40028 |
| H | 7.97588 | 15.10282 | -1.12273 |
| H | 6.38523 | 15.66005 | -0.56454 |
| H | 7.65288 | 16.83043 | -0.93089 |
| H | 7.32947 | 17.86813 | 1.31078 |
| H | 6.11536 | 16.65272 | 1.74983 |
| H | 7.51684 | 16.91732 | 2.79581 |
| H | 10.04148 | 15.43810 | 0.37614 |
| H | 9.61075 | 17.15481 | 0.47050 |
| H | 9.87877 | 16.22887 | 1.95128 |
| H | 6.68502 | 13.56511 | -0.00940 |
| H | 4.09527 | 10.24743 | 0.85146 |
| H | 4.63021 | 10.83799 | 2.43393 |
| H | 4.19227 | 11.99034 | 1.17077 |
| H | 5.62026 | 10.40365 | -1.15848 |
| H | 5.52606 | 12.14865 | -0.95370 |
| H | 7.10867 | 11.36075 | -1.08871 |
| H | 6.22170 | 8.88849 | 0.54015 |
| H | 7.81399 | 9.64048 | 0.76137 |
| H | 6.75798 | 9.37188 | 2.14723 |
| H | 7.34881 | 10.98268 | 3.34266 |
| H | 10.82202 | 12.12142 | 2.76687 |
| H | 10.39319 | 12.49673 | 0.51466 |
| H | 11.15809 | 12.08227 | -1.02940 |
| H | 9.78459 | 11.13569 | -0.42839 |
| H | 13.68017 | 10.83230 | 1.44830 |
| H | 13.43158 | 11.87870 | 0.03912 |
| H | 12.75259 | 12.33145 | 1.60602 |
| H | 12.76592 | 8.88770 | 0.04365 |
| H | 11.17630 | 9.03042 | -0.73431 |
| H | 12.52457 | 10.02659 | -1.28561 |
| H | 11.02180 | 8.10826 | 1.28220 |
| H | 9.51854 | 6.52756 | 1.19178 |
| H | 8.83473 | 5.27227 | 2.22967 |
| H | 8.06926 | 6.86958 | 2.14403 |
| H | 9.01910 | 5.35029 | 4.67150 |
| H | 9.73366 | 6.71723 | 5.52353 |
| H | 8.17696 | 6.90172 | 4.68680 |
| H | 11.80493 | 6.26281 | 2.39758 |
| H | 11.86679 | 6.33412 | 4.16539 |

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|---|---|---|---|
| H | 11.06988 | 4.97272 | 3.36043 |
| H | 9.41051 | 8.88454 | 5.17567 |
| H | 12.46405 | 10.87775 | 4.88628 |
| H | 15.77648 | 11.73264 | 5.26739 |
| H | 16.11830 | 10.69604 | 3.86904 |
| H | 14.52340 | 11.44066 | 4.05408 |
| H | 13.41930 | 9.08484 | 3.89162 |
| H | 15.04585 | 8.42246 | 3.66476 |
| H | 13.99736 | 7.79272 | 4.94651 |
| H | 16.61793 | 9.82531 | 6.73654 |
| H | 15.86427 | 8.22199 | 6.64134 |
| H | 16.84392 | 8.82351 | 5.29987 |
| H | 14.91442 | 9.61610 | 8.16262 |
| H | 12.63437 | 11.12702 | 12.12608 |
| H | 12.35265 | 12.26152 | 10.79523 |
| H | 11.33678 | 10.82061 | 10.97314 |
| H | 13.48878 | 8.80087 | 11.69237 |
| H | 12.27127 | 8.50846 | 10.43482 |
| H | 13.99056 | 8.30842 | 10.06741 |
| H | 14.95350 | 10.86764 | 11.60657 |
| H | 15.54615 | 10.33418 | 10.03432 |
| H | 14.88321 | 11.96254 | 10.21498 |
| H | 11.13375 | 11.48735 | 8.90303 |
| H | 12.57412 | 13.80555 | 7.11369 |
| H | 15.34336 | 17.23941 | 8.43618 |
| H | 13.89664 | 17.22146 | 7.41238 |
| H | 13.76601 | 17.65994 | 9.12041 |
| H | 14.48247 | 14.20609 | 10.47210 |
| H | 15.71469 | 15.44731 | 10.17822 |
| H | 14.17773 | 15.88363 | 10.93199 |
| H | 14.70753 | 13.58548 | 7.95134 |
| H | 14.50839 | 14.85281 | 6.72841 |
| H | 15.89754 | 14.88974 | 7.81731 |
| H | 12.14590 | 16.53700 | 10.38884 |
| H | 10.97583 | 16.20429 | 12.35371 |
| H | 9.32549 | 16.46439 | 12.93509 |
| H | 9.81859 | 14.87122 | 12.32320 |
| H | 9.32919 | 18.20843 | 9.60183 |
| H | 9.06089 | 18.42074 | 11.34159 |
| H | 10.69940 | 18.18813 | 10.72180 |
| H | 7.60198 | 16.33730 | 9.62666 |
| H | 7.75595 | 14.99124 | 10.76137 |
| H | 7.41062 | 16.61694 | 11.36379 |
| H | 8.71625 | 14.50713 | 8.79177 |
| H | 10.51523 | 15.81509 | 5.58236 |
| H | 10.51600 | 20.21995 | 3.98230 |

H 9.73546 18.81169 3.23914
H 8.80097 19.90513 4.26663
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H 9.22854 19.93058 6.82600
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H 12.27755 18.85012 4.98250
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H 11.61849 17.38182 4.25045
H 7.48761 18.84622 5.67892
H 5.37934 17.28211 8.27401
H 3.76037 16.97026 7.62129
H 4.97742 15.68170 7.64473
H 4.76268 16.79594 4.01247
H 4.58031 15.39300 5.06901
H 3.39880 16.70851 5.14357
H 5.57413 19.28151 6.72469
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H 3.97316 18.91064 6.07904
H 6.44317 14.70866 6.15477
H 6.83009 13.13027 7.41220
H 8.02998 12.09880 9.11537
C 9.82067 8.22501 8.83610
C 10.40448 7.26587 8.34870
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PhCCCCPh 1st ins. product
C 9.64948 5.09152 8.90641
C 10.36610 6.24093 8.52007
C 11.71421 6.10086 8.13463
C 12.32024 4.84921 8.14399
C 11.60072 3.71620 8.52489
C 10.26396 3.84426 8.90323
C 9.74287 7.51945 8.52011
C 9.21187 8.62322 8.56961
C 8.60173 9.87584 8.51324
C 8.21640 10.66630 9.54271
C 8.26008 10.50877 11.00081
C 7.81114 11.56289 11.81611
C 7.82016 11.45211 13.20223
C 8.27531 10.27964 13.80531
C 8.71831 9.22274 13.00905
C 8.71267 9.33079 11.62224
C 11.40813 6.01505 3.70973
C 10.04966 6.73088 3.57720
C 9.23113 6.44373 4.84101
C 10.28394 8.23362 3.35652
C 10.93635 8.65260 2.18583

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| C | 11.17963 | 9.99779 | 1.89750 |
| C | 10.72956 | 10.94796 | 2.82283 |
| C | 10.09370 | 10.57768 | 4.01275 |
| C | 9.88615 | 9.21408 | 4.27215 |
| C | 9.70611 | 11.66321 | 4.95987 |
| C | 8.82594 | 12.75803 | 4.63427 |
| C | 8.93086 | 13.71892 | 5.69782 |
| C | 9.88557 | 13.23386 | 6.64587 |
| C | 10.37848 | 11.96729 | 6.19080 |
| C | 10.44814 | 14.06613 | 7.74551 |
| C | 9.63288 | 14.65902 | 8.71692 |
| C | 10.16708 | 15.51109 | 9.68991 |
| C | 11.54373 | 15.75744 | 9.66096 |
| C | 12.39424 | 15.18848 | 8.70470 |
| C | 11.82443 | 14.33950 | 7.75202 |
| C | 13.89265 | 15.52931 | 8.72282 |
| C | 14.68004 | 14.74224 | 7.66640 |
| C | 9.30489 | 16.17006 | 10.77708 |
| C | 7.81544 | 15.84481 | 10.61132 |
| Th | 7.60619 | 11.45339 | 6.90400 |
| C | 5.04871 | 11.28163 | 5.80525 |
| C | 4.79585 | 11.58232 | 7.17518 |
| C | 5.16847 | 10.44773 | 7.95032 |
| C | 5.65516 | 9.44458 | 7.06945 |
| C | 5.58595 | 9.96009 | 5.74180 |
| C | 8.43070 | 15.12683 | 5.72024 |
| C | 7.10649 | 15.49251 | 5.95781 |
| C | 6.70825 | 16.84186 | 5.96059 |
| C | 7.68272 | 17.80955 | 5.71577 |
| C | 9.02784 | 17.48595 | 5.47380 |
| C | 9.37963 | 16.13836 | 5.48175 |
| C | 8.14707 | 12.95143 | 3.32028 |
| C | 8.09986 | 14.23041 | 2.75017 |
| C | 7.55193 | 14.46161 | 1.48267 |
| C | 7.04386 | 13.36969 | 0.78014 |
| C | 7.09006 | 12.06392 | 1.28934 |
| C | 7.63612 | 11.87565 | 2.56385 |
| C | 11.55666 | 11.26186 | 6.76987 |
| C | 12.58831 | 10.82461 | 5.93104 |
| C | 13.76627 | 10.26095 | 6.44064 |
| C | 13.88939 | 10.14513 | 7.82568 |
| C | 12.89226 | 10.59075 | 8.70794 |
| C | 11.73141 | 11.13816 | 8.15963 |
| C | 11.91684 | 10.45659 | 0.62951 |
| C | 12.36310 | 9.27791 | -0.24667 |
| C | 4.05303 | 12.77579 | 7.69660 |

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|---|---|---|---|
| C | 4.92118 | 10.28949 | 9.42067 |
| C | 5.98561 | 8.02608 | 7.42910 |
| C | 5.82134 | 9.15370 | 4.49801 |
| C | 4.63344 | 12.12855 | 4.63626 |
| C | 7.55636 | 15.88318 | 0.90077 |
| C | 9.00607 | 16.40305 | 0.83629 |
| C | 6.51800 | 10.90668 | 0.44953 |
| C | 7.11509 | 9.55076 | 0.85542 |
| C | 5.24746 | 17.21704 | 6.25510 |
| C | 4.98699 | 18.72433 | 6.11736 |
| C | 10.04634 | 18.61054 | 5.23775 |
| C | 11.44272 | 18.06840 | 4.90384 |
| C | 14.88422 | 9.83629 | 5.47616 |
| C | 16.10393 | 9.25677 | 6.20676 |
| C | 13.09511 | 10.44307 | 10.22489 |
| C | 14.53440 | 10.82021 | 10.62499 |
| C | 9.28379 | 6.14425 | 2.37423 |
| C | 10.99082 | 11.35650 | -0.20996 |
| C | 13.17258 | 11.25720 | 1.02655 |
| C | 4.90148 | 16.80350 | 7.69870 |
| C | 4.30985 | 16.49013 | 5.27334 |
| C | 9.58683 | 19.50052 | 4.06673 |
| C | 10.15431 | 19.46709 | 6.51497 |
| C | 6.96946 | 15.93957 | -0.51645 |
| C | 6.72083 | 16.80925 | 1.80430 |
| C | 4.98757 | 10.86490 | 0.63300 |
| C | 6.81587 | 11.10639 | -1.04994 |
| C | 15.35349 | 11.06448 | 4.67165 |
| C | 14.35279 | 8.76319 | 4.50827 |
| C | 12.13764 | 11.34312 | 11.01922 |
| C | 12.84184 | 8.97533 | 10.62048 |
| C | 14.07729 | 17.03401 | 8.44431 |
| C | 14.48696 | 15.20243 | 10.10657 |
| C | 9.76221 | 15.66988 | 12.16154 |
| C | 9.46395 | 17.70180 | 10.71063 |
| H | 7.44940 | 12.47552 | 11.34882 |
| H | 7.47022 | 12.28033 | 13.81233 |
| H | 8.28346 | 10.18929 | 14.88801 |
| H | 9.07121 | 8.30511 | 13.47202 |
| H | 9.05587 | 8.50395 | 11.01020 |
| H | 12.27176 | 6.98375 | 7.83822 |
| H | 13.36225 | 4.75755 | 7.84939 |
| H | 12.07841 | 2.74055 | 8.52766 |
| H | 9.69636 | 2.96703 | 9.20206 |
| H | 8.61044 | 5.19177 | 9.20510 |
| H | 5.64819 | 9.75675 | 3.60552 |

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| H | 6.83520 | 8.74231 | 4.42660 |
| H | 5.13107 | 8.30176 | 4.45444 |
| H | 5.30342 | 12.02856 | 3.77854 |
| H | 3.62393 | 11.85565 | 4.30058 |
| H | 4.60395 | 13.19045 | 4.89395 |
| H | 4.38698 | 13.05735 | 8.69791 |
| H | 4.17933 | 13.64984 | 7.05392 |
| H | 2.97550 | 12.56706 | 7.74915 |
| H | 5.06201 | 11.22807 | 9.96459 |
| H | 3.88859 | 9.96311 | 9.60330 |
| H | 5.58277 | 9.54618 | 9.87118 |
| H | 5.10330 | 7.38336 | 7.30364 |
| H | 6.77983 | 7.61054 | 6.80240 |
| H | 6.31447 | 7.93466 | 8.46660 |
| H | 8.52327 | 15.06026 | 3.30151 |
| H | 7.53527 | 15.31841 | -1.21920 |
| H | 5.92275 | 15.61763 | -0.53838 |
| H | 7.00291 | 16.96993 | -0.88599 |
| H | 6.73217 | 17.83415 | 1.41482 |
| H | 5.67890 | 16.47353 | 1.84278 |
| H | 7.10391 | 16.83416 | 2.82821 |
| H | 9.62491 | 15.76131 | 0.20002 |
| H | 9.02836 | 17.41682 | 0.41957 |
| H | 9.46816 | 16.43900 | 1.82697 |
| H | 6.61585 | 13.53058 | -0.20125 |
| H | 4.54813 | 10.06156 | 0.02969 |
| H | 4.71347 | 10.69009 | 1.67798 |
| H | 4.52958 | 11.81041 | 0.32396 |
| H | 6.47784 | 10.22844 | -1.61125 |
| H | 6.29632 | 11.97190 | -1.47107 |
| H | 7.88720 | 11.23407 | -1.23217 |
| H | 6.74294 | 8.76788 | 0.18566 |
| H | 8.20764 | 9.55899 | 0.79769 |
| H | 6.83970 | 9.25999 | 1.87160 |
| H | 7.70159 | 10.87529 | 2.97585 |
| H | 10.88095 | 12.00672 | 2.63341 |
| H | 10.64101 | 12.22541 | 0.35428 |
| H | 11.51920 | 11.72070 | -1.09870 |
| H | 10.10952 | 10.80098 | -0.54507 |
| H | 13.86285 | 10.64123 | 1.61166 |
| H | 13.70155 | 11.60088 | 0.13019 |
| H | 12.92233 | 12.14063 | 1.62183 |
| H | 13.05242 | 8.61306 | 0.28456 |
| H | 11.51256 | 8.68363 | -0.59760 |
| H | 12.88579 | 9.65556 | -1.13176 |
| H | 11.26754 | 7.89596 | 1.48320 |

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| H | 8.23261 | 6.89050 | 4.78413 |
| H | 9.10023 | 5.36290 | 4.95697 |
| H | 9.72173 | 6.81010 | 5.74653 |
| H | 11.25886 | 4.93662 | 3.83606 |
| H | 12.03440 | 6.16637 | 2.82506 |
| H | 11.95889 | 6.38376 | 4.57997 |
| H | 8.31878 | 6.64388 | 2.24055 |
| H | 9.84313 | 6.24266 | 1.43919 |
| H | 9.09407 | 5.07676 | 2.53427 |
| H | 9.42538 | 8.92321 | 5.21202 |
| H | 12.47843 | 10.95105 | 4.86009 |
| H | 15.74600 | 11.84077 | 5.33681 |
| H | 16.14936 | 10.78188 | 3.97225 |
| H | 14.53846 | 11.50402 | 4.08976 |
| H | 13.48579 | 9.11427 | 3.94158 |
| H | 15.13229 | 8.47507 | 3.79278 |
| H | 14.04856 | 7.86439 | 5.05476 |
| H | 16.55757 | 9.98473 | 6.88775 |
| H | 15.84854 | 8.36092 | 6.78299 |
| H | 16.86705 | 8.97041 | 5.47506 |
| H | 14.79246 | 9.71175 | 8.23880 |
| H | 12.36135 | 11.26724 | 12.08878 |
| H | 12.23443 | 12.39341 | 10.72511 |
| H | 11.09328 | 11.04827 | 10.89032 |
| H | 12.97512 | 8.84022 | 11.70054 |
| H | 11.82433 | 8.66944 | 10.36027 |
| H | 13.53663 | 8.30115 | 10.10850 |
| H | 14.64043 | 10.77275 | 11.71450 |
| H | 15.28032 | 10.14149 | 10.20080 |
| H | 14.78472 | 11.83628 | 10.30422 |
| H | 10.94152 | 11.49126 | 8.81017 |
| H | 12.44226 | 13.87761 | 6.99078 |
| H | 15.14032 | 17.30122 | 8.47280 |
| H | 13.68772 | 17.30070 | 7.45670 |
| H | 13.55774 | 17.64957 | 9.18541 |
| H | 14.36263 | 14.14260 | 10.34794 |
| H | 15.55862 | 15.43246 | 10.12328 |
| H | 14.01334 | 15.78259 | 10.90425 |
| H | 14.58212 | 13.66122 | 7.80894 |
| H | 14.35086 | 14.98348 | 6.65013 |
| H | 15.74353 | 14.99527 | 7.73487 |
| H | 11.97103 | 16.41956 | 10.40957 |
| H | 10.81250 | 15.91130 | 12.35247 |
| H | 9.16326 | 16.13515 | 12.95348 |
| H | 9.65063 | 14.58375 | 12.24224 |
| H | 9.14092 | 18.08514 | 9.73743 |

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|---|---|---|---|
| H | 8.85419 | 18.18145 | 11.48534 |
| H | 10.50079 | 18.01503 | 10.86655 |
| H | 7.43168 | 16.18731 | 9.64570 |
| H | 7.62218 | 14.77017 | 10.68433 |
| H | 7.23836 | 16.34086 | 11.39929 |
| H | 8.57006 | 14.44307 | 8.68938 |
| H | 10.40598 | 15.83731 | 5.30465 |
| H | 10.31349 | 20.30279 | 3.89468 |
| H | 9.49726 | 18.91963 | 3.14324 |
| H | 8.61782 | 19.96971 | 4.26146 |
| H | 10.87107 | 20.28364 | 6.36800 |
| H | 9.19184 | 19.91314 | 6.78502 |
| H | 10.49395 | 18.86235 | 7.36165 |
| H | 12.13267 | 18.90330 | 4.74130 |
| H | 11.84628 | 17.45868 | 5.71817 |
| H | 11.43667 | 17.46170 | 3.99181 |
| H | 7.39650 | 18.85532 | 5.71766 |
| H | 5.50954 | 17.36176 | 8.41806 |
| H | 3.84678 | 17.01102 | 7.91464 |
| H | 5.07946 | 15.73823 | 7.86979 |
| H | 4.53106 | 16.77051 | 4.23877 |
| H | 4.40132 | 15.40342 | 5.34876 |
| H | 3.26551 | 16.74936 | 5.48208 |
| H | 5.57894 | 19.30996 | 6.82856 |
| H | 5.20529 | 19.08610 | 5.10676 |
| H | 3.93169 | 18.93308 | 6.32226 |
| H | 6.38312 | 14.71192 | 6.17447 |
| H | 6.99668 | 13.08041 | 8.01202 |
| H | 7.73666 | 11.64946 | 9.29230 |

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PhCCCCPh 2nd ins. Product

| | | | |
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| C | 9.48046 | 1.09176 | 7.64671 |
| C | 10.06760 | -0.07138 | 8.20164 |
| C | 10.99140 | -0.78322 | 8.65623 |
| C | 12.32383 | -1.09089 | 9.02188 |
| C | 12.65014 | -1.61029 | 10.36674 |
| C | 13.95338 | -2.06434 | 10.63714 |
| H | 14.69959 | -2.02264 | 9.84723 |
| C | 14.29842 | -2.56912 | 11.88623 |
| H | 15.31529 | -2.91019 | 12.06388 |
| C | 13.34814 | -2.64402 | 12.90612 |
| H | 13.61675 | -3.03761 | 13.88223 |
| C | 12.04327 | -2.22773 | 12.64534 |
| H | 11.28280 | -2.30583 | 13.41851 |
| C | 11.69624 | -1.72765 | 11.39174 |
| H | 10.66722 | -1.44101 | 11.19095 |

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|---|---|---|---|
| C | 8.28571 | 1.70261 | 8.26570 |
| C | 7.74030 | 1.23635 | 9.47393 |
| H | 8.19779 | 0.38129 | 9.96521 |
| C | 6.60919 | 1.83010 | 10.03002 |
| H | 6.20939 | 1.44702 | 10.96575 |
| C | 5.97937 | 2.89407 | 9.38579 |
| H | 5.09427 | 3.35352 | 9.81637 |
| C | 6.48984 | 3.34495 | 8.16723 |
| H | 5.99673 | 4.15910 | 7.64164 |
| C | 7.62275 | 2.75731 | 7.61399 |
| H | 8.00900 | 3.11030 | 6.66050 |
| C | 11.65015 | 2.35291 | 10.64145 |
| C | 13.05897 | 2.16386 | 10.54739 |
| C | 13.57064 | 3.13206 | 9.63607 |
| C | 12.47887 | 3.91663 | 9.16406 |
| C | 11.29175 | 3.43587 | 9.78850 |
| C | 10.74328 | 1.71624 | 11.65330 |
| H | 9.72603 | 1.59207 | 11.27458 |
| H | 11.10853 | 0.73749 | 11.96896 |
| H | 10.67921 | 2.34662 | 12.55047 |
| C | 13.90577 | 1.30560 | 11.43899 |
| H | 14.70952 | 0.79636 | 10.89993 |
| H | 14.37715 | 1.92314 | 12.21616 |
| H | 13.32171 | 0.53312 | 11.94054 |
| C | 15.02899 | 3.41936 | 9.42571 |
| H | 15.52643 | 2.76197 | 8.70154 |
| H | 15.57597 | 3.31275 | 10.36887 |
| H | 15.16829 | 4.44899 | 9.08586 |
| C | 12.57237 | 5.18273 | 8.36388 |
| H | 11.57883 | 5.57389 | 8.13858 |
| H | 13.09439 | 5.95847 | 8.93985 |
| H | 13.10864 | 5.07109 | 7.41635 |
| C | 9.96760 | 4.13903 | 9.78131 |
| H | 9.16535 | 3.50432 | 10.15943 |
| H | 10.01555 | 5.03111 | 10.42027 |
| H | 9.66561 | 4.46882 | 8.78450 |
| C | 14.10725 | 0.98761 | 5.86704 |
| C | 13.31315 | 2.11118 | 5.44037 |
| C | 12.00930 | 1.61561 | 5.07635 |
| C | 12.02372 | 0.18806 | 5.22890 |
| C | 13.31462 | -0.20169 | 5.71924 |
| C | 15.59100 | 1.01961 | 6.03835 |
| C | 16.24878 | 0.59354 | 7.19478 |
| H | 15.65467 | 0.24573 | 8.03740 |
| C | 17.65429 | 0.57371 | 7.27703 |
| C | 18.35199 | 0.09290 | 8.56025 |

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|---|---|---|---|
| C | 17.92879 | 0.97637 | 9.74795 |
| H | 18.20153 | 2.02302 | 9.57705 |
| H | 16.85041 | 0.93364 | 9.92137 |
| H | 18.42437 | 0.64132 | 10.66628 |
| C | 19.88253 | 0.15054 | 8.45335 |
| H | 20.26188 | -0.49065 | 7.65075 |
| H | 20.24244 | 1.17029 | 8.27979 |
| H | 20.32734 | -0.19979 | 9.39060 |
| C | 17.95132 | -1.36636 | 8.84603 |
| H | 18.27325 | -2.02440 | 8.03320 |
| H | 18.41969 | -1.71669 | 9.77294 |
| H | 16.86911 | -1.47807 | 8.95437 |
| C | 18.37719 | 0.98689 | 6.15748 |
| H | 19.46070 | 0.97378 | 6.19767 |
| C | 17.75871 | 1.40769 | 4.96779 |
| C | 18.62555 | 1.80188 | 3.76006 |
| C | 19.51366 | 0.61138 | 3.34806 |
| H | 18.90657 | -0.24677 | 3.04606 |
| H | 20.15027 | 0.89193 | 2.50095 |
| H | 20.16936 | 0.28820 | 4.16224 |
| C | 19.53324 | 2.99067 | 4.12957 |
| H | 18.93915 | 3.87791 | 4.36733 |
| H | 20.16959 | 2.76873 | 4.99167 |
| H | 20.18947 | 3.24136 | 3.28808 |
| C | 17.77914 | 2.20881 | 2.54666 |
| H | 17.13968 | 3.06911 | 2.76795 |
| H | 18.43715 | 2.48726 | 1.71662 |
| H | 17.14289 | 1.38692 | 2.20123 |
| C | 16.36610 | 1.42498 | 4.93411 |
| H | 15.84515 | 1.73853 | 4.03741 |
| C | 13.89486 | 3.41571 | 4.99992 |
| C | 14.81704 | 4.14923 | 5.75831 |
| H | 15.04278 | 3.81177 | 6.76323 |
| C | 15.48310 | 5.27180 | 5.23411 |
| C | 16.48286 | 6.08444 | 6.07736 |
| C | 17.39194 | 5.16237 | 6.90781 |
| H | 17.96633 | 4.48694 | 6.26858 |
| H | 18.09853 | 5.76411 | 7.49044 |
| H | 16.83215 | 4.54598 | 7.61355 |
| C | 15.70007 | 7.01298 | 7.02637 |
| H | 15.04443 | 7.68636 | 6.46404 |
| H | 15.07545 | 6.44273 | 7.71858 |
| H | 16.38925 | 7.62525 | 7.61994 |
| C | 17.39542 | 6.96424 | 5.20569 |
| H | 16.84411 | 7.75930 | 4.69357 |
| H | 18.14339 | 7.45203 | 5.83960 |

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|---|---|---|---|
| H | 17.92806 | 6.37563 | 4.45134 |
| C | 15.18483 | 5.64826 | 3.92386 |
| H | 15.69072 | 6.50574 | 3.49510 |
| C | 14.26554 | 4.95061 | 3.12708 |
| C | 14.02621 | 5.40945 | 1.68020 |
| C | 15.33503 | 5.27082 | 0.87748 |
| H | 16.14187 | 5.87314 | 1.30683 |
| H | 15.67095 | 4.22918 | 0.85328 |
| H | 15.18492 | 5.60276 | -0.15655 |
| C | 13.58454 | 6.88572 | 1.66687 |
| H | 14.33631 | 7.54430 | 2.11219 |
| H | 13.41900 | 7.22221 | 0.63697 |
| H | 12.65071 | 7.02118 | 2.22073 |
| C | 12.94259 | 4.58045 | 0.97946 |
| H | 11.98584 | 4.63077 | 1.50875 |
| H | 12.78622 | 4.96244 | -0.03527 |
| H | 13.22862 | 3.52713 | 0.89227 |
| C | 13.63458 | 3.83840 | 3.68152 |
| H | 12.94460 | 3.25611 | 3.08429 |
| C | 10.94144 | 2.42228 | 4.41680 |
| C | 10.55374 | 3.68792 | 4.90233 |
| H | 11.00697 | 4.05308 | 5.81912 |
| C | 9.63181 | 4.48287 | 4.21630 |
| C | 9.20128 | 5.88452 | 4.67800 |
| C | 9.83522 | 6.28097 | 6.01392 |
| H | 9.54399 | 5.59275 | 6.81380 |
| H | 10.92745 | 6.30271 | 5.95130 |
| H | 9.50004 | 7.28287 | 6.30229 |
| C | 7.66927 | 5.93938 | 4.83926 |
| H | 7.14796 | 5.71596 | 3.90395 |
| H | 7.32771 | 5.22198 | 5.59177 |
| H | 7.35894 | 6.94008 | 5.16106 |
| C | 9.63360 | 6.92046 | 3.62155 |
| H | 9.19230 | 6.71440 | 2.64191 |
| H | 9.32155 | 7.92677 | 3.92409 |
| H | 10.72194 | 6.92292 | 3.50623 |
| C | 9.09138 | 3.98315 | 3.02055 |
| H | 8.38113 | 4.59779 | 2.47903 |
| C | 9.44100 | 2.73783 | 2.50369 |
| C | 8.85751 | 2.20249 | 1.18759 |
| C | 9.99936 | 1.89775 | 0.19958 |
| H | 10.70329 | 1.16467 | 0.60281 |
| H | 9.59359 | 1.49161 | -0.73425 |
| H | 10.56160 | 2.80536 | -0.04244 |
| C | 7.90669 | 3.20308 | 0.51562 |
| H | 7.04045 | 3.43253 | 1.14539 |

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|---|---|---|---|
| H | 8.41095 | 4.14304 | 0.26619 |
| H | 7.52691 | 2.77573 | -0.41844 |
| C | 8.06989 | 0.91073 | 1.47391 |
| H | 7.23384 | 1.11186 | 2.15216 |
| H | 7.65896 | 0.49993 | 0.54422 |
| H | 8.69677 | 0.14204 | 1.93429 |
| C | 10.36809 | 1.96889 | 3.22248 |
| H | 10.67328 | 1.00381 | 2.83542 |
| C | 11.09731 | -0.78378 | 4.55586 |
| C | 11.59541 | -1.40092 | 3.40060 |
| H | 12.60690 | -1.15753 | 3.08772 |
| C | 10.83823 | -2.31568 | 2.65738 |
| C | 11.44845 | -2.96985 | 1.40830 |
| C | 11.84428 | -1.87986 | 0.39360 |
| H | 12.57446 | -1.18001 | 0.81149 |
| H | 12.29283 | -2.33327 | -0.49795 |
| H | 10.96940 | -1.30365 | 0.07553 |
| C | 10.47374 | -3.93189 | 0.71508 |
| H | 10.17964 | -4.75824 | 1.37077 |
| H | 9.56557 | -3.42111 | 0.37719 |
| H | 10.95363 | -4.36820 | -0.16741 |
| C | 12.70480 | -3.76573 | 1.81126 |
| H | 13.45039 | -3.13178 | 2.29911 |
| H | 12.45211 | -4.56954 | 2.50927 |
| H | 13.16909 | -4.21596 | 0.92595 |
| C | 9.54511 | -2.59948 | 3.10332 |
| H | 8.93773 | -3.30522 | 2.54702 |
| C | 9.00299 | -2.00918 | 4.25487 |
| C | 7.57609 | -2.37730 | 4.69597 |
| C | 7.12838 | -1.59499 | 5.93795 |
| H | 7.12842 | -0.51413 | 5.76446 |
| H | 6.10685 | -1.88494 | 6.20578 |
| H | 7.76543 | -1.79912 | 6.80436 |
| C | 7.50815 | -3.88129 | 5.02696 |
| H | 7.79641 | -4.50129 | 4.17233 |
| H | 8.17131 | -4.13088 | 5.86066 |
| H | 6.48683 | -4.15933 | 5.31202 |
| C | 6.58294 | -2.07178 | 3.55762 |
| H | 6.81331 | -2.63354 | 2.64712 |
| H | 5.56534 | -2.34082 | 3.86352 |
| H | 6.59017 | -1.00720 | 3.30582 |
| C | 9.79772 | -1.10667 | 4.96910 |
| H | 9.40632 | -0.66427 | 5.87221 |
| C | 13.77719 | -1.61920 | 5.77672 |
| C | 12.91949 | -2.64429 | 6.20188 |
| H | 11.91196 | -2.38623 | 6.51076 |

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|---|---|---|---|
| C | 13.31469 | -3.99028 | 6.22126 |
| C | 12.34318 | -5.07357 | 6.71425 |
| C | 11.81636 | -4.71541 | 8.11642 |
| H | 11.26240 | -3.77293 | 8.12211 |
| H | 11.13783 | -5.49852 | 8.47391 |
| H | 12.63617 | -4.62368 | 8.83580 |
| C | 13.00470 | -6.45658 | 6.80031 |
| H | 13.86154 | -6.45716 | 7.48283 |
| H | 12.27949 | -7.18463 | 7.17878 |
| H | 13.34303 | -6.81350 | 5.82159 |
| C | 11.15914 | -5.16651 | 5.73459 |
| H | 10.65045 | -4.20516 | 5.62463 |
| H | 11.49627 | -5.47770 | 4.74029 |
| H | 10.42729 | -5.90202 | 6.08924 |
| C | 14.59194 | -4.29646 | 5.75578 |
| H | 14.91918 | -5.33016 | 5.75359 |
| C | 15.46796 | -3.31544 | 5.26958 |
| C | 16.82773 | -3.75465 | 4.70561 |
| C | 17.66605 | -2.56684 | 4.22198 |
| H | 17.16406 | -2.02570 | 3.41275 |
| H | 17.87357 | -1.85529 | 5.02704 |
| H | 18.62627 | -2.92445 | 3.83480 |
| C | 16.60287 | -4.69891 | 3.50755 |
| H | 16.04829 | -4.19368 | 2.71015 |
| H | 17.56431 | -5.02881 | 3.09660 |
| H | 16.03807 | -5.59196 | 3.79167 |
| C | 17.62728 | -4.50182 | 5.79068 |
| H | 17.10280 | -5.39488 | 6.14337 |
| H | 18.59845 | -4.82157 | 5.39532 |
| H | 17.80755 | -3.85889 | 6.65768 |
| C | 15.05142 | -1.98327 | 5.29928 |
| H | 15.70626 | -1.20707 | 4.92587 |
| Th | 12.10446 | 1.37597 | 8.00668 |
| H | 12.86408 | -1.63880 | 8.24761 |
| H | 9.40473 | 1.08037 | 6.55699 |

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